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NUCLEAR PROPERTIES FOR ASTROPHYSICAL APPLICATIONS*

P. MÖLLER

Theoretical Division, Los Alamos National Laboratory
Los Alamos, NM 87545
and
Center for Mathematical Sciences, University of Aizu
Aizu-Wakamatsu, Fukushima 965-80, Japan

J. R. NIX

Theoretical Division, Los Alamos National Laboratory
Los Alamos, NM 87545

and

K.-L. KRATZ

Institut für Kernchemie, Universität Mainz
D-55099 Mainz, Germany

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We tabulate the ground-state odd-proton and odd-neutron spins and parities, proton and neutron pairing gaps, binding energy, one- and two-neutron separation energies, quantities related to β-delayed one- and two-neutron emission probabilities, β-decay energy release and half-life with respect to Gamow-Teller decay, one- and two-proton separation energies, and α-decay energy release and half-life for 8979 nuclei ranging from ^{16}O to $^{339}136$ and extending from the proton drip line to the neutron drip line. Single-particle level diagrams and other quantities are also presented in graphical form. The starting point of our present work is a study of nuclear ground-state masses and deformations based on the finite-range droplet model and folded-Yukawa single-particle potential published in a previous issue of Atomic Data and Nuclear Data Tables. The β-delayed neutron-emission probabilities and Gamow-Teller β-decay rates are obtained from a quasi-particle random-phase approximation with single-particle levels and wave functions at the calculated nuclear ground-state shapes as input quantities.

*This paper is dedicated to the memory of our friend and colleague Vilen M. Strutinsky, who through his years of devoted research on nuclear-structure models, most notably the Strutinsky shell-correction method, made possible many of the calculations discussed here.

Contents

1 INTRODUCTION

In a previous issue of Atomic Data and Nuclear Data Tables we presented a calculation of nuclear ground-state masses and deformations for 8979 nuclei ranging from ^{16}O to ^{339}136 and extending from the proton drip line to the neutron drip line.[1]) The 1992 version of the finite-range droplet model and folded-Yukawa single-particle potential that was the basis for this calculation is referred to as the FRDM (1992). We here use these ground-state masses and deformations as starting points for calculations of additional ground-state properties that are useful for astrophysical and other applications.

An important feature of a mass model is its reliability for nuclei beyond the region used for the determination of the model constants. In particular, can one expect the model to be reliable for nuclei very far from β-stability and in the region of superheavy elements? In our mass paper[1]) we addressed the model reliability for new regions of nuclei by comparing predictions of masses that were not included in the data set to which the model constants were determined to new experimental data. Since at that time we had available very few new masses over and

above the 1989 data set [2]) from which the model constants were determined, we had to test model reliability by simulation. In one simulation, where the model was adjusted to a 1977 experimental data set, it was found that 351 new masses measured between 1977 and 1989 were calculated with an increase of only 2% in the model error. In another simulation, where we adjusted the model constants only to nuclei in the region $Z, N \geq 28$ and $A \leq 208$, we found that there was no increase in the *mean* error but some increase in the standard deviation for nuclei beyond $A = 208$ that were not included in the limited adjustment. However, for superheavy nuclei such as $^{288}110$ and $^{290}110$, the difference in mass predictions between the FRDM (1992), whose constants were determined by including nuclei up to $A = 263$, and the limited adjustment was only of the order of 1 MeV. It is significant that these superheavy nuclei are 80 mass units heavier than the heaviest nuclide included in the limited adjustment.

Because our previous studies indicated a very good model reliability for new regions of nuclei, we here present calculations of additional nuclear ground-state properties based on the same model and the same values of model constants, for the same set of 8979 nuclei considered in our mass calculation. [1]) Specifically, we consider the following quantities:

Odd-nucleon spins and parities:

Projection of the odd-proton angular momentum along the symmetry axis and parity of the wave function	$\Omega_{\rm p}^{\pi}$
Projection of the odd-neutron angular momentum along the symmetry axis and parity of the wave function	$\Omega_{\rm n}^{\pi}$

Lipkin-Nogami pairing gaps:

Proton pairing gap	$\Delta_{\rm LN_p}$
Neutron pairing gap	$\Delta_{\rm LN_n}$

FRDM mass-related quantity:

Total binding energy	$E_{\rm bind}$

Neutron separation energies:

One-neutron separation energy	$S_{\rm 1n}$
Two-neutron separation energy	$S_{\rm 2n}$

Beta-decay properties:

Probability for producing a final nucleus with mass number A following β decay and delayed neutron emission	P_A
Probability for producing a final nucleus with mass number $A-1$ following β decay and delayed neutron emission	P_{A-1}
Probability for producing a final nucleus with mass number $A-2$ following β decay and delayed neutron emission	P_{A-2}
Energy released in β decay	Q_β
Half-life with respect to Gamow-Teller β decay	T_β

Proton separation energies:

One-proton separation energy	S_{1p}
Two-proton separation energy	S_{2p}

Alpha-decay properties:

Energy released in α decay	Q_α
Half-life with respect to α decay	T_α

The details of the calculations are given in Sec. 2. Separation energies and energy releases are readily obtained from mass differences. The β-decay half-lives and β-delayed neutron-emission probabilities are obtained from a quasi-particle random-phase approximation (QRPA). In the QRPA the single-particle energies and wave functions at the calculated ground-state deformation serve as the starting point. The tabulated results are described in Sec. 3.

After the submission of our mass paper [1]) a new mass evaluation [3,4]) has become available. It contains 217 new masses that were not included in the 1989 data set [2]) from which the values of the FRDM (1992) constants were determined. Therefore, we are now able to assess the reliability, without simulations, of the FRDM (1992) and of several other models that are also commonly used in astrophysical calculations. These reliability issues are discussed in Sec. 4.

As one particular application, we discuss in Sec. 5 the use of the calculated quantities in astrophysical *rp*- and *r*-process calculations. However, our results also have wider applicability to several other areas of astrophysics and to such fields as reactor physics. Section 6 contains calculated proton and neutron single-particle level diagrams for representative spherical and deformed nuclei throughout the periodic system.

2 CALCULATIONAL DETAILS

The quantities studied in this paper are obtained in four different ways.

1. The odd-proton spin and parity Ω_p^π, odd-neutron spin and parity Ω_n^π, proton pairing gap Δ_{LN_p}, and neutron pairing gap Δ_{LN_n} are microscopic quantities obtained simultaneously with the calculated ground-state masses and deformations. They were not published in our mass paper because of space limitations.

2. The total binding energy E_{bind}, one-neutron separation energy S_{1n}, two-neutron separation energy S_{2n}, β-decay energy release Q_β, one-proton separation energy S_{1p}, two-proton separation energy S_{2p}, and α-decay energy release Q_α are obtained from appropriate differences of the calculated mass excesses. For convenient access we publish them here.

3. The β-delayed occupation probabilities P_A, P_{A-1}, and P_{A-2} and β-decay half-lives T_β are obtained from a microscopic quasi-particle random-phase approximation (QRPA).

4. The α-decay half-life T_α is obtained from the semi-empirical relationship of Viola and Seaborg, [5]) with constants determined by Sobiczewski, Patyk, and Čwiok. [6])

2.1 Odd-nucleon spin and parity

The odd-nucleon spin is simply the projection of the angular momentum along the symmetry axis (Ω quantum number) for the last occupied proton or neutron level, when this level is occupied

by a single nucleon. For odd-proton or odd-neutron nuclei the spin of the nucleus is simply $\Omega_{\rm p}$ or $\Omega_{\rm n}$, respectively. The superscript π gives the parity of the wave function.

For spherical nuclei with degenerate levels, the nuclear spin is defined as the maximum value of j_z, which is $|j|$. Thus, for a spherical nucleus we cannot use as an odd-even spin assignment the Ω value automatically provided for the last occupied single-particle level, since this level is randomly assigned any Ω value in the range 1/2 to $|j|$. For slightly deformed nuclei one could in principle use deformed assignments, but in practice it would be unrealistic to list a deformed assignment for a nucleus with a calculated deformation of, say, $\epsilon_2 = 0.01$. We therefore proceed in the following manner. For nuclei with a deformation $|\epsilon_2| \geq \epsilon_{\rm crit}$ a deformed assignment is used. For nuclei with $|\epsilon_2| < \epsilon_{\rm crit}$ we calculate the levels for a spherical shape and adopt the spherical spin assignment thus obtained. When we compare below in Sec. 3.1 calculated odd-particle spins and parities with experimental data, we show that the results are quite insensitive to the exact value of $\epsilon_{\rm crit}$. We choose here

$$\epsilon_{\rm crit} \quad = \quad 0.15$$

For nuclei whose ground states are calculated to have the octupole shape parameter $\epsilon_3 \neq 0$ parity is not conserved and is therefore not tabulated.

2.2 Pairing gaps

In an extensive study of nuclear pairing [7]) we investigated both a macroscopic pairing model and a microscopic pairing model, which was solved in both the BCS [8–11]) and Lipkin-Nogami (LN) [12–14]) approximations. For each model we determined a preferred form of the effective pairing interaction and optimum values of the constants of the effective pairing interaction, which were obtained from a least-squares minimization of the difference between calculated pairing gaps and experimental odd-even mass differences.

An important result of our previous study is that it is crucial to differentiate between several pairing-gap concepts. The most simple concept is the *average* pairing gap $\overline{\Delta}$, which is an algebraic relationship such as $c/\sqrt{A}$, where c is a constant and A is the number of nucleons in the system being studied. The average pairing gap may be regarded as a macroscopic model for the nuclear pairing gap, and it may therefore be directly compared with experimental odd-even mass differences.

When a microscopic approach is used the situation is considerably more complicated. In this case the quantities that are compared to experimental odd-even mass differences are obtained as solutions to microscopic pairing equations, for example the BCS or LN equations. In the BCS method it is Δ that should be directly compared to the odd-even mass differences. However, in the LN approximation it is the sum of the pairing gap Δ and the number-fluctuation constant λ_2, where Δ and λ_2 are obtained as solutions of the LN equations, that should be compared to odd-even mass differences. We denote this sum by $\Delta_{\rm LN}$. Thus, $\Delta_{\rm LN} = \Delta + \lambda_2$.

To solve the usual pairing equations [7]) one needs in addition to single-particle energies also the value of the pairing-strength constant G. This constant depends in a complicated way on the number of levels included in the calculation and on the particular nuclear region considered. However, it may be determined from an effective-interaction pairing gap Δ_G by use of a Strutinsky-like procedure. [7]) At first sight this may seem an unnecessary complication, but the advantage is that Δ_G does not depend on the particular truncation of the single-particle level spectrum that is chosen in the calculation. Furthermore, it depends in a very simple way on Z and N. Therefore, a significant simplification is achieved if one considers Δ_G to be the primary input quantity for pairing calculations, with the constants that enter the function that defines Δ_G to be the pairing-model effective-interaction constants.

In our earlier study [7]) we obtained the following preferred functional form for the effective-interaction pairing gap Δ_G:

$$\Delta_{G\mathrm{p}} = \frac{rB_\mathrm{s}}{Z^{1/3}} e^{-tI^2}$$
$$\Delta_{G\mathrm{n}} = \frac{rB_\mathrm{s}}{N^{1/3}} e^{-tI^2} \tag{1}$$

Here Z and N are the numbers of protons and neutrons, respectively, $I = (N - Z)/(N + Z)$ is the relative neutron excess, and B_s is the surface area of the nucleus divided by the surface area of the spherical shape. From root-mean-square minimizations we obtained results consistent with $t = 0$ for both the BCS and LN models. For these cases Eq. (1) simplifies to

$$\Delta_{G\mathrm{p}} = \frac{rB_\mathrm{s}}{Z^{1/3}}$$
$$\Delta_{G\mathrm{n}} = \frac{rB_\mathrm{s}}{N^{1/3}} \tag{2}$$

and the effective-interaction pairing gap Δ_G is determined by one constant for the entire nuclear chart, for both protons and neutrons.

In our nuclear mass calculation [1]) we performed a refined determination of the effective pairing-interaction constant r, with the result that we adopted the value $r = 3.2$ MeV instead of the earlier value [7]) $r = 3.3$ MeV. For details we refer to these earlier studies. [1,7]) Although we revised the effective-interaction pairing constant r by 3%, the earlier extensive pairing study [7]) can still serve as an excellent guide to the properties of our current pairing model. Below we present further results obtained in the current model.

2.3 Total binding energy

The total binding energy $E_\mathrm{bind}(Z, N)$ is related to the atomic mass excess $M(Z, N)$ through the simple relationship

$$E_\mathrm{bind} = ZM_\mathrm{H} + NM_\mathrm{n} - M(Z, N) \tag{3}$$

where M_H is the hydrogen-atom mass excess and M_n is the neutron mass excess. The total binding energy includes the binding energy of the Z electrons comprising the atom, which we approximate by $a_\mathrm{el}Z^{2.39}$, with $a_\mathrm{el} = 1.433 \times 10^{-5}$ MeV.

For the benefit of workers in other fields, who are often confused by the conventions adopted in atomic masses, we mention that the reason that the atomic mass excess is tabulated instead of the atomic mass itself is simply to eliminate the repetitive tabulation of additional leading numbers that can easily be restored by adding the mass number A times the mass unit u, which is 1/12 the mass of the ^{12}C atom, to the tabulated quantity. Also, the reason that the atomic mass is considered rather than the nuclear mass is that the former is the actual experimentally measured quantity, whereas the latter is less accurate because its extraction requires a knowledge of the binding energy of the Z atomic electrons.

For those applications where it is necessary to know the actual mass of the nucleus itself, its value (in MeV) can be found from the atomic mass excess tabulated in Ref. [1]) by use of the relationship

$$M_\mathrm{nucleus} = A\mathrm{u} + M - Zm_\mathrm{e} + a_\mathrm{el}Z^{2.39} \tag{4}$$

where $m_\mathrm{e} = 0.51099906$ MeV is the mass of the electron. [15,16]) As discussed in Ref. [1]), the value u = 931.5014 MeV that was used in the interim 1989 mass evaluation [2]) should be used for the atomic mass unit in Eq. (4).

2.4 Neutron separation energies

The one- and two-neutron separation energies $S_{1n}(Z,N)$ and $S_{2n}(Z,N)$ are obtained from the mass excesses through the differences

$$\begin{aligned} S_{1n}(Z,N) &= M(Z,N-1) + M_n - M(Z,N) \\ S_{2n}(Z,N) &= M(Z,N-2) + 2M_n - M(Z,N) \end{aligned} \tag{5}$$

2.5 β-decay properties

The formalism we use to calculate Gamow-Teller (GT) β-strength functions is fairly lengthy, since it involves adding pairing and Gamow-Teller residual interactions to the folded-Yukawa single-particle Hamiltonian and solving the resulting Schrödinger equation in the quasi-particle random-phase approximation. Because this model has been completely described in two previous papers,[17,18]) we refer to those two publications for a full model specification and for a definition of notation used. We restrict the discussion here to an overview of features that are particularly relevant to the results discussed in this paper.

It is well known that wave functions and transition matrix elements are more affected by small perturbations to the Hamiltonian than are the eigenvalues. When transition rates are calculated it is therefore necessary to add residual interactions to the folded-Yukawa single-particle Hamiltonian in addition to the pairing interaction that is included in the mass model. Fortunately, the residual interaction may be restricted to a term specific to the particular type of decay considered. To obtain reasonably accurate half-lives it is also very important to include ground-state deformations. Originally the QRPA formalism was developed for and applied only to spherical nuclei.[19,20]) The extension to deformed nuclei, which is necessary in global calculations of β-decay properties, was first described in 1984.[17])

To treat Gamow-Teller β decay we therefore add the Gamow-Teller force

$$V_{GT} = 2\chi_{GT} : \boldsymbol{\beta^{1-}} \cdot \boldsymbol{\beta^{1+}} : \tag{6}$$

to the folded-Yukawa single-particle Hamiltonian, after pairing has already been incorporated, with the standard choice $\chi_{GT} = 23$ MeV$/A$.[17–20]) Here $\boldsymbol{\beta^{1\pm}} = \sum_i \boldsymbol{\sigma_i} t_i^{\pm}$ are the Gamow-Teller $\beta^{\pm}$-transition operators, and the colans mean that all contractions in the quasi-particle representations of the enclosed operator are to be ignored. The correlations generated by the GT force are of specific importance to the Gamow-Teller decays, which are the dominant decay modes in many nuclei of astrophysical interest. Other types of residual interactions are of importance for other decay modes, but leave the Gamow-Teller decay rates unaffected, and can consequently be ignored for our present purpose.

It should be noted that the RPA treatment formulated by Halbleib and Sorensen[20]) incorporates only particle-hole correlations of specific importance to GT transitions. It has been proposed[21,22]) that the effect of neglected particle-particle terms may be significant for β^+ transitions. We later address this question in Sec. 3.5. Moreover, the RPA treatment may not contain enough ground-state correlations.[22]) However, in view of the present uncertainties regarding these points we leave possible further refinements for future consideration. Some additional comments are made in Sec. 3.5.

We next discuss the calculation of β-decay half-lives for Gamow-Teller decay and the related problem of calculating β-delayed neutron-emission probabilities. In our discussion of the model we use, unless otherwise stated, expressions and notation from the books by deShalit and Feshbach[23]) and Preston[24]) and from our previous publications.[17,18])

2.5.1 β^- and β^+ decay

The process of β decay occurs from an initial ground state or excited state in a mother nucleus to a final state in the daughter nucleus. For β^- decay, the final configuration is a nucleus in some excited state or its ground state, an electron (with energy E_e), and an antineutrino (with energy E_ν). The transition from the initial to the final state then involves an operator H, which is the weak-interaction Hamiltonian density. Once the operator H is known, the probability per unit time for emitting an electron with momentum between $\hbar\boldsymbol{k}_\mathrm{e}$ and $\hbar(\boldsymbol{k}_\mathrm{e}+d\boldsymbol{k}_\mathrm{e})$ and an antineutrino with momentum between $\hbar\boldsymbol{k}_\nu$ and $\hbar(\boldsymbol{k}_\nu+d\boldsymbol{k}_\nu)$ is given by the well-known Golden Rule

$$dw_{fi} = \frac{2\pi}{\hbar}|H_{fi}|^2 \frac{d\boldsymbol{k}_e}{(2\pi)^3}\frac{d\boldsymbol{k}_\nu}{(2\pi)^3}\,\delta(E_0 - E_\mathrm{e} - E_\nu) \tag{7}$$

where E_0 is the energy released in the decay.

In the above expression one should sum over the spins of the final states and average over the initial spins. Our interest here is mainly to obtain the probability of decay to a specific final nuclear state f. To obtain this probability one must go through several lengthy steps. These steps are usually glossed over in discussions of these models, but one fairly extensive account of these steps is given in the book by Preston.[24]) The final expression obtained through these steps for the total probability for decay to one nuclear state is

$$w_{fi} = \frac{m_0c^2}{\hbar}\,\frac{\Gamma^2}{2\pi^3}\,|M_{fi}|^2 f(Z,R,\epsilon_0) \tag{8}$$

where $\epsilon_0 = E_0/m_0c^2$, with m_0 the electron mass. For consistency with standard treatments of β decay we here use SI units. Moreover, $|M_{fi}|^2$ is the nuclear matrix element, which is also the β-strength function. The dimensionless constant Γ is defined by

$$\Gamma \equiv \frac{g}{m_0c^2}\left(\frac{m_0c}{\hbar}\right)^3 \tag{9}$$

where g is the Gamow-Teller coupling constant. There is a misprint concerning this quantity in the book[23]) by deShalit and Feshbach, where in their Chapter 9, Eq. (2.11) the exponent is erroneously given as 2 instead of the correct value 3. The quantity $f(Z,R,\epsilon_0)$ has been extensively discussed and tabulated elsewhere.[23–25])

For the special case in which the two-neutron separation energy S_2n in the daughter nucleus is greater than the energy Q_β released in the decay, the probability for β-delayed one-neutron emission, in percent, is given by

$$P_\mathrm{1n} = 100\,\frac{\sum\limits_{S_\mathrm{1n}<E_f<Q_\beta} w_{fi}}{\sum\limits_{0<E_f<Q_\beta} w_{fi}} \tag{10}$$

where E_f is the excitation energy in the daughter nucleus and S_1n is the one-neutron separation energy in the daughter nucleus. We assume that decays to energies above S_1n always lead to delayed neutron emission. In the more general case where multiple-neutron emission is energetically possible, but under the restriction that $S_{\nu\mathrm{n}}$ in the daughter nucleus monotonically increase with increasing ν, we define

$$P^{>}_{\nu\mathrm{n}} = 100\,\frac{\sum\limits_{S_{\nu\mathrm{n}}<E_f<Q_\beta} w_{fi}}{\sum\limits_{0<E_f<Q_\beta} w_{fi}} \tag{11}$$

where $P^{>}_{\nu\mathrm{n}}$ is the probability of emitting ν or more neutrons. The occupation probabilities $P_{A-\nu}$ introduced above are then given by

$$\begin{aligned} P_A &= 100 - P^{>}_{1\mathrm{n}} \\ P_{A-\nu} &= P^{>}_{\nu\mathrm{n}} - P^{>}_{(\nu+1)\mathrm{n}} \end{aligned} \tag{12}$$

For some very neutron-rich nuclei $S_{\nu\mathrm{n}}$ no longer monotonically increase with increasing ν, in which case the above formalism cannot be used. In the Table we present calculated values only when the above formalism is valid and otherwise put "..." in the columns for $P_{A-\nu}$.

To obtain the half-life with respect to β-decay one sums up the decay rates w_{fi} to the individual nuclear states in the allowed energy window. The half-life is then related to the total decay rate by

$$T_\beta = \frac{\ln 2}{\sum\limits_{0<E_f<Q_\beta} w_{fi}} \tag{13}$$

The above equation may be rewritten as

$$T_\beta = \frac{\hbar}{m_0c^2}\,\frac{2\pi^3 \ln 2}{\Gamma^2}\,\frac{1}{\sum\limits_{0<E_f<Q_\beta} |M_{fi}|^2 f(Z,R,\epsilon_0)} = \frac{B}{\sum\limits_{0<E_f<Q_\beta} |M_{fi}|^2 f(Z,R,\epsilon_0)} \tag{14}$$

with

$$B = \frac{\hbar}{m_0c^2}\,\frac{2\pi^3 \ln 2}{\Gamma^2} \tag{15}$$

For the value of B corresponding to Gamow-Teller decay we use

$$B = 4131 \text{ s} \tag{16}$$

The energy released in electron emission is

$$Q_{\beta^-} = E_0^{\beta^-} = [M(Z,N) - M(Z+1,N-1)]\,c^2 \tag{17}$$

whereas the energy released in positron emission is

$$Q_{\beta^+} = E_0^{\beta^+} = [M(Z,N) - M(Z-1,N+1) - 2m_0]\,c^2 \tag{18}$$

The above formulas apply to β^- and β^+ decay. However, for calculating half-lives electron capture (EC) must also be considered.

2.5.2 Electron capture

The energy released in electron capture is

$$Q_{\mathrm{EC}} = E_0^{\mathrm{EC}} = [M(Z,N) - M(Z-1,N+1)]\,c^2 - \text{electron binding energy} \tag{19}$$

so that

$$E_0^{\mathrm{EC}} = E_0^{\beta^+} + 2m_0c^2 - \text{electron binding energy} \tag{20}$$

This shows that for some decays electron capture is possible whereas β^+ decay is energetically forbidden. The total probability for decay to one nuclear state is again given by Eq. (8), where the final state f now refers to electron capture over all electron shells *or* to β^+ decay.

The total half-life with respect to β^+ and EC decay is given by

$$T_\beta = \frac{\ln 2}{\left(\sum\limits_{0<E_f<Q_{\rm EC}} w_{fi}^{\rm EC} + \sum\limits_{0<E_f<Q_{\beta^+}} w_{fi}^{\beta^+} \right)} \tag{21}$$

As pointed out above, the energies involved in the two terms in the sum differ by $2m_0c^2$ minus the electron binding energy and for some nuclear final states $w_{fi}^{\beta^+}$ may be zero (energetically forbidden) while $w_{fi}^{\rm EC}$ is not.

To obtain an initial feel for these models we first studied the approximate relativistic expressions given by Preston.[24]) The results obtained by use of these expressions for β^- decay are typically within 20% of those obtained in the more exact treatment by Gove and Martin,[25]) who have made extensive tabulations of $f(Z, R, \epsilon_0)$. Despite the small differences we have obtained the computer code used to generate the tables of Gove and Martin and incorporated it into our programs. The results presented here have been obtained with this more accurate treatment.

In the Table we present five quantities related to β decay, namely P_A, P_{A-1}, P_{A-2}, Q_β, and T_β. The precise meaning of these quantities is as follows. When both β^+ and β^- decay are possible, we tabulate $\pm$ in the columns for Q_β and T_β. When neither β^+ nor β^- decay is possible, we tabulate "..." in the column for Q_β, "β-stable" in the column for T_β, and blank fields in the columns for P_A, P_{A-1}, and P_{A-2}. When only EC or β^+ decay is possible, we tabulate $Q_{\rm EC}$ in the column for Q_β, the calculated half-life with respect to Gamow-Teller decay for combined EC and β^+ decay in the column for T_β, and blank fields in the columns for P_A, P_{A-1}, and P_{A-2}. Finally, when only β^- decay is possible, we tabulate Q_{β^-} in the column for Q_β, the calculated half-life with respect to Gamow-Teller β^- decay in the column for T_β, and the calculated occupation probabilities after β-delayed neutron emission in the columns for P_A, P_{A-1}, and P_{A-2}. The electron binding energy has been neglected in the determination of $Q_{\rm EC}$.

To obtain more accurate values of T_β and $P_{\nu{\rm n}}$, we have calculated the Q values that enter Eqs. (11), (13), and (21) from experimental mass differences when all experimental masses that are required for the calculation are available and otherwise from calculated mass differences. The neutron separation energies that enter in the calculations of $P_{\nu{\rm n}}$ in Eq. (11) are also obtained from experimental mass differences when available and otherwise from calculated mass differences. Calculated deformations are always used, even when experimental data are available. However, in the astrophysical applications presented below, further use is made of experimental information, as is discussed in Sec. 5.

2.6 Proton separation energies

The one- and two-proton separation energies $S_{1{\rm p}}(Z,N)$ and $S_{2{\rm p}}(Z,N)$ are obtained from mass excesses through the differences

$$\begin{aligned} S_{1{\rm p}}(Z,N) &= M(Z-1,N) + M_{\rm H} - M(Z,N) \\ S_{2{\rm p}}(Z,N) &= M(Z-2,N) + 2M_{\rm H} - M(Z,N) \end{aligned} \tag{22}$$

2.7 α-decay properties

The five heaviest known elements 107, 108, $_{109}$Mt, 110, and 111 were all identified from their α-decay chains,[26–30]) which limited their stability. The neutron number of the first identified isotope of 108 and Mt was $N = 157$. Because α-decay chains provide very clear signatures of the nuclear species in the beginning of the decay chain and fission does not, it is likely that additional new nuclei discovered in the heaviest region will often be identified through their

α-decay properties. Models of α-decay properties are therefore highly useful for designing and interpreting experiments that explore the limits of stability of the heaviest elements. Obviously, one also needs to consider whether spontaneous-fission half-lives are significantly shorter than the α-decay half-lives. In that case spontaneous-fission would be the dominating decay mode and α decay might not be detected.

The single most important quantity determining the α-decay half-life is the energy release Q_α. In the heavy-element region an uncertainty of 1 MeV in Q_α corresponds to an uncertainty of $10^{\pm 5}$ for $Q_\alpha \approx 7$ MeV and to an uncertainty of $10^{\pm 3}$ for $Q_\alpha \approx 9$ MeV.[31]) The energy release Q_α is obtained from the mass excesses through the difference

$$Q_\alpha(Z,N) = M(Z,N) - M(Z-2,N-2) - M(2,2) \tag{23}$$

The α-decay half-lives T_α presented in the Table are estimated by use of the Viola-Seaborg relationship[5])

$$\log(T_\alpha/\mathrm{s}) = (aZ+b)(Q_\alpha/\mathrm{MeV})^{-1/2} + (cZ+d) \tag{24}$$

where Z is the proton number of the parent nucleus. Instead of using the original set of constants suggested by Viola and Seaborg we use the more recent values

$$\begin{aligned} a &= +1.66175, \quad b = -8.5166 \\ c &= -0.20228, \quad d = -33.9069 \end{aligned}$$

that were determined in an adjustment taking into account new data for even-even nuclei.[6]) The uncertainties in the calculated half-lives due to this semi-empirical approach are far smaller than uncertainties due to errors in the calculated energy release.

3 TABULATED RESULTS

Deformed single-particle models provide the starting point for the calculations of nuclear ground-state masses and deformations, which were extensively discussed in our previous paper.[1]) Since nuclear wave functions are also provided by these models, one may also use these models to determine electromagnetic moments and transition rates, β-strength functions, β-decay half-lives, and β-delayed neutron-emission probabilities.

The results of our calculations of many such nuclear properties for astrophysical applications are presented in the Table. To provide an overview of these results, we present in Figs. 1–16 color diagrams of the calculated pairing gaps, neutron separation energies, proton separation energies, α-decay energy release and half-life, β-decay half-life, and some related quantities. Beyond $Z \approx 120$ and $N \approx 190$ the calculated potential-energy surfaces on which Figs. 1–16 are based are very flat and the barrier with respect to fission is almost zero. Because the ground state is identified as the deepest local pocket in this flat surface, one obtains rapidly fluctuating deformations, separation energies, and energy releases between neighboring nuclei. These results are of no physical significance, since the spontaneous-fission half-life of these nuclei will be much too short to allow experimental observation.

3.1 Odd-nucleon spin and parity

The most important constants in the folded-Yukawa single-particle model are the diffuseness and spin-orbit constants, which were determined[32]) in 1974 in the rare-earth and actinide regions from comparisons between calculated and experimental single-particle level orderings. The global nuclear-mass study[33]) in 1981 introduced a set of constants valid for the entire nuclear chart in terms of an expression for the spin-orbit strength that is linear in $A = N + Z$, with the expression fully defined by the previously determined values in the actinide and rare-earth

regions. This procedure is somewhat subjective because it is not based on exact comparisons between all available experimental data and calculations. Instead, one typically proceeds by calculating single-particle level diagrams as functions of deformation for several sets of constants, comparing their structure to a few selected nuclei, and choosing the set that gives the best agreement.

Because we now have available nuclear ground-state shapes from our calculations of ground-state masses, we are in a position to compare calculated and experimental ground-state spins and parities in a well-defined manner, as shown in Figs. 17 and 18. The only ambiguity concerns the comparison for nuclei calculated to be weakly deformed. We have chosen to base the comparison on spherical assignments if $|\epsilon_2| < 0.15$ in the calculations. With this choice we obtain agreement in 446 cases and disagreement in 267 cases, corresponding to 63% agreement. When the ground-state energy is *not* minimized with respect to ϵ_3 and ϵ_6, we obtained in a previous calculation, as expected, slightly less favorable results: agreement in 428 cases and disagreement in 285 cases, corresponding to 60% agreement. These results are not very sensitive to changes in the choice concerning when to use spherical assignments. In the present study, if we *always* choose the spherical assignment when this choice yields agreement with experimental data, we obtain agreement in 482 cases and disagreement in 231 cases, corresponding to 68% agreement, so that the improvement in the agreement is only 5%.

The disagreements between the calculated and experimental spins and parities usually arise because several deformed or spherical levels lie very close together, making accurate calculations difficult. For magic numbers there is an almost stunning agreement, which, taken together with our analysis of the disagreements in other regions, makes it unlikely that a significantly better *global* set of constants can be found. The existing disagreements probably arise from residual interactions outside the framework of the single-particle model.

3.2 Pairing gaps

We first emphasize the most important results of our previous pairing study: [7])

1. The preferred form of the pairing gap given by Eq. (2) lowers the rms deviation by about 20% relative to the rms deviation obtained with the standard choice $c/\sqrt{A}$ for the average pairing-gap $\overline{\Delta}$ or effective-interaction pairing gap Δ_G.

2. The Lipkin-Nogami pairing model yields an rms deviation that is 14% lower than the rms deviation in the BCS approximation.

3. One cannot deduce the optimum constants for a microscopic pairing model by simplified macroscopic calculations.

4. It is necessary to distinguish between several pairing-gap concepts, notably the average pairing gap $\overline{\Delta}$, the effective-interaction pairing gap Δ_G used as input in microscopic calculations, and the microscopic pairing gap Δ obtained as a solution to the BCS or Lipkin-Nogami pairing equations.

5. The effective-interaction pairing-gap Δ_G does not depend explicitly on the relative neutron excess I.

Our first four color figures represent results of theoretical calculations of pairing quantities in the Lipkin-Nogami approximation. In this model a pairing gap Δ and number-fluctuation constant λ_2 are obtained as solutions of the pairing equations. It is the sum $\Delta + \lambda_2$, which we denote by $\Delta_{\rm LN}$, that should be compared to odd-even mass differences. This quantity is shown in Fig. 1 for protons. The areas enclosed in jagged black lines are regions where experimental pairing gaps can be extracted from experimental masses by use of fourth-order finite-difference

Table 1: Errors of pairing-gap calculations. The experimental data base contains 1654 masses.[2])

		LN				Mass model			
Nucleons	$N_{\rm nuc}$	$\mu_{\rm th}$ (MeV)	$\sigma_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	rms (MeV)	$\mu_{\rm th}$ (MeV)	$\sigma_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	rms (MeV)
Neutrons	756	0.0220	0.1610	0.1627	0.1712	−0.0427	0.1929	0.1972	0.2088
Protons	648	0.0455	0.1529	0.1596	0.1670	−0.0096	0.1728	0.1730	0.1994
Total	1404	0.0328	0.1577	0.1613	0.1692	−0.0274	0.1846	0.1865	0.2045

expressions. Because magic numbers and the $N = Z$ Wigner cusp give non-smooth contributions to the mass surface and corresponding contributions to the finite-difference expressions, it is not possible to extract experimental pairing gaps from mass differences in certain regions near magic numbers and near $N = Z$.[7,34]) The proton pairing gap $\Delta_{\rm LN_p}$ on the whole decreases with increasing A and with increasing Z. There is a decrease in the individual contribution $\Delta_{\rm p}$, which is not shown or tabulated in this paper, at magic proton numbers. This decrease is compensated for by a strong increase in $\lambda_{\rm 2p}$, which results in a smooth appearance of $\Delta_{\rm LN_p}$ at magic proton numbers.

The calculated neutron pairing gap $\Delta_{\rm LN_n}$ is shown in Fig. 2. The regions for neutrons where experimental pairing gaps can be extracted from odd-even mass differences are slightly different from those for protons shown in Fig. 1. The individual contribution $\Delta_{\rm n}$ decreases considerably near magic neutron numbers. This decrease is compensated for by a strong increase in $\lambda_{\rm 2n}$, so that their sum behaves relatively smoothly at magic neutron numbers, as seen in Fig. 2. The pairing gap $\Delta_{\rm LN_n}$ on the whole decreases with increasing A and with increasing N. There is no collapse at magic neutron numbers, in contrast to results based on the BCS approximation.

As discussed in our previous pairing study,[7]) one may also determine pairing gaps directly from odd-even mass differences based on *theoretical* masses. This type of theoretical pairing gap we denote by $\Delta_{\rm thmass}$. There are several strong reasons to expect that it is more appropriate to compare $\Delta_{\rm thmass}$ to $\Delta_{\rm exp}$ than to compare $\Delta_{\rm LN}$ to $\Delta_{\rm exp}$. The odd-even mass differences pick up any non-smooth contributions to the nuclear-mass surface, in addition to those represented by the pairing gaps. Although we have excluded regions near magic numbers from consideration, there are other gaps in the level spectra that are expected to give non-smooth contributions in the odd-even mass differences. These include the $N = 56$ spherical subshell near the proton gap at $Z = 40$ and the $N = 152$ deformed gap near the proton gap at $Z = 100$ in the actinide region. Shape transitions also give rise to non-smooth components to odd-even mass differences. Such additional contributions to $\Delta_{\rm exp}$ are expected near $N = 88$ in the transition to the deformed rare-earth region, for example. Figures 3 and 4 clearly exhibit discrepancies related to these gaps and shape transitions that *cannot* automatically be interpreted as an inherent deficiency of the microscopic pairing model.

These non-smooth contributions should be equally present in both $\Delta_{\rm exp}$ and $\Delta_{\rm thmass}$, provided that the theoretical calculation accurately describes the nuclear mass surface. Although neither $\Delta_{\rm exp}$ nor $\Delta_{\rm thmass}$ represent the true pairing gap because of these non-smooth contributions, they should cancel out in the discrepancy $\Delta_{\rm exp} - \Delta_{\rm thmass}$. In Table 1 we present a study of the two discrepancies $\Delta_{\rm exp} - \Delta_{\rm LN}$ and $\Delta_{\rm exp} - \Delta_{\rm thmass}$. In contrast to our expectations, we find better agreement between $\Delta_{\rm exp}$ and $\Delta_{\rm LN}$ than between $\Delta_{\rm exp}$ and $\Delta_{\rm thmass}$. The total second central moment is 16% larger in the latter comparison than in the former. The reason that we

obtain such a large error for $\Delta_{\rm thmass}$ is that the deviation of the calculated mass surface from the true mass surface is sufficiently large to cancel the advantages of using $\Delta_{\rm thmass}$ as a theoretical pairing gap instead of $\Delta_{\rm LN}$. In the transition regions between spherical and deformed nuclei near magic numbers, where we had expected such advantages, the error in the calculated mass surface is especially large, as can be seen in the comparison of measured and calculated masses in Fig. 19.

3.3 Total binding energy

The total binding energy is equivalent to the atomic mass excess, which has been discussed extensively in our mass paper.[1]) It is listed in the Table to facilitate applications that require binding energy rather than mass excess.

3.4 Neutron separation energies

One- and two-neutron separation energies are shown versus N and Z in Figs. 5–7. The r-process takes place primarily in the region 2.0 MeV $< S_{\rm 1n} <$ 3.0 MeV for odd N. Near $N = 50$ and $N = 82$ the region of known nuclei extends into the r-process region.

The discrepancy between experimental one-neutron separation energies obtained from mass differences and calculated one-neutron separation energies is shown in Fig. 8. The biggest errors occur near magic numbers. There is a general decrease of the error as A increases.

3.5 β-decay properties

A detailed knowledge of the low-energy part of the β-strength function is essential for the calculation of many nuclear-structure quantities of astrophysical interest, such as the probability of β-delayed neutron and proton emission, the probability of β-delayed fission, and half-lives with respect to β decay. Experimentally it has been known for some time that the low-energy part of the β-strength function exhibits a pronounced structure,[35,36]) where the strength is collected in a few well-localized peaks. For nuclei that are spherical in their ground state there are usually only a few peaks within the Q_β window; for deformed nuclei the strength is more spread out, but still exhibits significant structure.

Theoretically, these main features of the β-strength function can be understood on the basis of an extreme single-particle model. The peaks in the strength functions correspond to transitions between specific single-particle levels. In the spherical case the levels are highly degenerate and spaced far apart, which gives rise to very few but strong peaks in the experimental strength function. For deformed nuclei the degeneracy is removed, allowing for significantly more transitions. Thus, compared to the spherical case, there are now more peaks in the experimental strength function, but the strength of each peak is lower.

Although an extreme single-particle model explains the origin of the structure in the β-strength function and the characteristic difference between strength functions associated with deformed and spherical nuclei, a more detailed description of the strength function requires the consideration of the residual pairing and Gamow-Teller interactions discussed above. The inclusion of these terms in the potential reduces the calculated strength in the low-energy part of the strength function to about 10% of what is obtained in an extreme single-particle model.[17]) Because pairing leads to a diffuse Fermi surface and consequently to some occupation probability above and to partially unfilled levels below the Fermi surface, there are decay channels open in the more refined model that are blocked in the extreme single-particle model. For deformed nuclei one often finds considerable strength for transitions between Nilsson levels whose asymptotic quantum numbers do not allow for any transition probability according to the GT selection rules. This occurs because the conventional, asymptotic quantum-number label gives the main

component of the wave function corresponding to the level, but the transition strength is due to small admixtures of wave functions with other asymptotic quantum numbers. Since we perform a full diagonalization of the single-particle Hamiltonian we account for these admixtures in our model.

The β-strength function is a sensitive measure of the underlying single-particle structure. Therefore, when calculating a β-strength function, two conditions should ideally be fulfilled. First, the ground-state shape of the system of interest must be known. Second, the single-particle spectrum calculated at this shape must agree reasonably well with the experimental situation, especially for the levels closest to the Fermi surface. The calculation of a β-decay half-life also requires the energy released in the decay, or equivalently the ground-state masses of the mother and daughter nuclei. We now use the folded-Yukawa single-particle potential, which has been applied to the calculation of nuclear masses, shapes, and other ground-state quantities for nuclei throughout the periodic system, [1,33,37]) where these requirements are met globally. We noted in Sec. 3.1 that for spherical nuclei there was excellent agreement between calculated and measured ground-state spins and parities. For deformed regions disagreements occurred somewhat more often. However, when a disagreement occurs, a level with the correct spin and parity is often calculated to be very near the last occupied orbital. If this situation occurs in the daughter nucleus there is a rather small effect on the calculated β-strength function. If, however, in a decay from an odd-even or odd-odd nucleus the unpaired proton or neutron is in an incorrect level the effect can be more significant. Therefore, it is reasonable to expect characteristic differences in the discrepancies between calculated and experimental half-lives in odd-even and even-even decay. Surprisingly, as will be discussed below, we see no such differences.

To illustrate some major features associated with β-decay we show in Figs. 20 and 21 calculated β-strength functions for the spherical nucleus ^{95}Rb and the deformed nucleus ^{99}Rb. Although we obtain a fairly large deformation for ^{95}Rb in our calculation of nuclear ground-state masses and deformations [1]) we have performed the calculation shown in Fig. 20 for a spherical shape, which is consistent with experimental information on this nucleus, so that we can study β-strength-function features associated with a sudden onset of deformation as the neutron number increases from $N = 58$ to $N = 62$. As discussed in more detail in Ref. [18]), the single-particle and pairing properties are evaluated for the appropriate vacuum nucleus. In addition, the Q_β value corresponds to the decay indicated and the $S_{\nu\mathrm{n}}$ and $P_{\nu\mathrm{n}}$ are evaluated for the daughter of the decay. A characteristic difference between β-strength functions of spherical and deformed nuclei is that the former contain only a few strong peaks in the low-energy region, whereas the latter contain many more peaks of smaller size. Therefore, the likelihood that one or several of them will occur close to zero energy is much larger in the deformed case than in the spherical case. Because the transition rate is proportional to $S_\beta(E_x - Q_\beta)^5$, where E_x is the excitation energy of the daughter state, there is therefore usually a characteristic drop in the β-decay half-life at the transition from a spherical to a deformed system.

It is not our aim here to make a detailed analysis of each individual nucleus, but instead to present an overview of the model performance in a calculation of a large number of β-decay half-lives. In Figs. 22–27 we compare measured and calculated β-decay half-lives for nuclei throughout the periodic system. The experimental half-lives are from a compilation by Browne. [38]) We present results with respect to β^- decay and also to β^+ decay and electron capture. To avoid lengthy constructions we will in our discussion in this section usually not distinguish between β^+ decay and electron capture and somewhat inexactly take Q_β to mean the maximum energy release in the decay. Because the calculated pairing gap affects o-o, o-e, and e-e decays differently we analyze these decays separately to differentiate between effects due to pairing and due to other causes.

We have limited the comparison to nuclei whose experimental half-lives are shorter than 1000 s. Because the relative error in the calculated half-lives is more sensitive to small shifts in

the positions of the calculated single-particle levels for decays with small energy releases, where long half-lives are expected, one can anticipate that half-life calculations are more reliable far from stability than close to β-stable nuclei. To address the reliability in various regions of nuclei and versus distance from stability, we present in Figs. 22–27 the ratio $T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}}$ versus the *three* different quantities N, $T_{\beta,\mathrm{exp}}$, and Q_β.

The few cases that lie outside the scale of the figures have been taken into account in the error analysis presented below. These cases are associated with long experimental half-lives; there is only one case outside the scale of the figure with an experimental half-life less than 10 s. In such cases first-forbidden transitions, which we do not take into account at this stage, can be expected to make a considerable contribution to the decay rate. Therefore, one should not conclude from these relatively few very large deviations that the calculated *Gamow-Teller* β-strength function is in serious disagreement with experimental data.

Before we make a quantitative analysis of the agreement between calculated and experimental half-lives we briefly discuss what conclusions can be drawn from a simple visual inspection of Figs. 22–27. In Figs. 22 and 25 the quantities $T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}}$ are plotted as functions of neutron number N. There are no systematic trends with N. For β^- decay of even-even nuclei the calculated half-lives are somewhat too long on the average. In Figs. 23 and 26 the quantities $T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}}$ are plotted as functions of the experimental half-life $T_{\beta,\mathrm{exp}}$. As a function of this quantity, one would expect the average error to increase as $T_{\beta,\mathrm{exp}}$ increases. This is indeed the case for β^- decay, but not for β^+ decay, except for odd-odd decays—an unexpected result. In Figs. 24 and 27 the quantities $T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}}$ are plotted as functions of Q_β with the aim of showing how the average error increases as Q_β decreases. It is obvious that errors in the location of the peaks in the calculated strength function have a larger effect on the calculated half-lives for small values of Q_β than for larger ones. Indeed, we see a fairly clear increase in the scatter of the points in Fig. 24 as Q_β decreases. However, for β^+ decay shown in Fig. 27 the only correlation occurs for o-o decay.

In a visual inspection of Figs. 22–27 one is left with the impression that the errors in our calculation are fairly large. However, this is partly a fallacy, since for small errors there are many more points than for large errors. This is not clearly seen in the figures, since for small errors many points are superimposed on one another. To obtain a more exact understanding of the error in the calculation we therefore perform a more detailed analysis.

One often analyzes the error in a calculation by studying a root-mean-square deviation, which in this case would be

$$\sigma_{\mathrm{rms}}{}^2 = \frac{1}{n}\sum_{i=1}^{n}(T_{\beta,\mathrm{exp}} - T_{\beta,\mathrm{calc}})^2 \tag{25}$$

However, such an error analysis is unsuitable here, for two reasons. First, the quantities studied vary by many orders of magnitude. In our case the variation is more than ten orders of magnitude, from the millisecond range to years and beyond. Second, the calculated and measured quantities may *differ* by orders of magnitude. We therefore study the quantity $\log(T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}})$, which is plotted in Figs. 22–27, instead of $(T_{\beta,\mathrm{exp}} - T_{\beta,\mathrm{calc}})^2$.

To facilitate the interpretation of the error plots we consider two hypothetical cases. As the first example, suppose that all the points were grouped on the line $T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}} = 10$. It is immediately clear that an error of this type could be entirely removed by introducing a renormalization factor, which is a common practice in the calculation of β-decay half-lives. We shall see below that in our model the half-lives corresponding to our calculated strength functions have about zero average deviation from the calculated half-lives, so no renormalization factor is necessary.

In another extreme, suppose half the points were located on the line $T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}} = 10$ and the other half on the line $T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}} = 0.1$. In this case the average of $\log(T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}})$ would be zero. We are therefore led to the conclusion that there are two types of errors that are

of interest to study, namely the average position of the points in Figs. 22–27, which is just the average of the quantity $\log(T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}})$, and the spread of the points around this average. To analyze the error along these ideas, we introduce the quantities

$$\begin{aligned} r &= T_{\beta,\mathrm{calc}}/T_{\beta,\mathrm{exp}} \\ r_{\mathrm{l}} &= \log_{10}(r) \\ M_{r_{\mathrm{l}}} &= \frac{1}{n}\sum_{i=1}^{n} r_{\mathrm{l}}^{i} \\ M_{r_{\mathrm{l}}}^{10} &= 10^{M_{r_{\mathrm{l}}}} \\ \sigma_{r_{\mathrm{l}}} &= \left[\frac{1}{n}\sum_{i=1}^{n}\left(r_{\mathrm{l}}^{i} - M_{r_{\mathrm{l}}}\right)^{2}\right]^{1/2} \\ \sigma_{r_{\mathrm{l}}}^{10} &= 10^{\sigma_{r_{\mathrm{l}}}} \end{aligned} \tag{26}$$

where $M_{r_{\mathrm{l}}}$ is the average position of the points and $\sigma_{r_{\mathrm{l}}}$ is the spread around this average. The spread $\sigma_{r_{\mathrm{l}}}$ can be expected to be related to uncertainties in the positions of the levels in the underlying single-particle model. The use of a logarithm in the definition of r_{l} implies that these two quantities correspond directly to distances as seen by the eye in Figs. 22–27, in units where one order of magnitude is 1. After the error analysis has been carried out we want to discuss its result in terms like "on the average the calculated half-lives are 'a factor of two' too long." To be able to do this we must convert back from the logarithmic scale. Thus, we realize that the quantities $M_{r_{\mathrm{l}}}^{10}$ and $\sigma_{r_{\mathrm{l}}}^{10}$ are conversions back to "factor of" units of the quantities $M_{r_{\mathrm{l}}}$ and $\sigma_{r_{\mathrm{l}}}$, which are expressed in distance or logarithmic units.

In Table 2 we show the results of an evaluation of the quantities in Eq. (26) for β^- decay of nuclei with $T_{\beta,\mathrm{exp}} \leq 1000$ s. For long half-lives one expects forbidden decay to dominate.

Table 2: Analysis of the discrepancy between calculated and measured β^--decay half-lives shown in Fig. 23.

	n	$M_{r_{\mathrm{l}}}$	$M_{r_{\mathrm{l}}}^{10}$	$\sigma_{r_{\mathrm{l}}}$	$\sigma_{r_{\mathrm{l}}}^{10}$	$T_{\beta,\mathrm{exp}}^{\mathrm{max}}$ (s)
o-o	29	−0.23	0.59	0.46	2.91	1
o-e	35	−0.23	0.59	0.42	2.64	1
e-e	10	0.58	3.84	0.49	3.08	1
o-o	59	−0.12	0.76	0.95	8.83	10
o-e	85	−0.11	0.78	0.68	4.81	10
e-e	34	0.40	2.50	0.62	4.13	10
o-o	88	0.37	2.33	1.69	49.19	100
o-e	133	0.05	1.11	0.98	9.45	100
e-e	54	0.42	2.61	0.68	4.75	100
o-o	115	0.54	3.50	1.86	72.02	1000
o-e	194	0.44	2.77	1.85	71.50	1000
e-e	71	0.84	6.86	1.77	58.48	1000

We find that in the o-o and o-e cases the value of $M_{r_1}^{10}$ increases from values somewhat below 1 to values somewhat above 1 as the maximum half-life, $T_{\beta,\mathrm{exp}}^{\mathrm{max}}$, considered increases from 1 s to 1000 s. When cases corresponding to long half-lives contribute to the error estimates, first-forbidden decays would be expected to increase the β-decay rates. In our model we neglect, at this stage, first-forbidden decay. Therefore, one can expect that as $T_{\beta,\mathrm{exp}}^{\mathrm{max}}$ increases, our calculated half-lives will become increasingly longer than experiment. This is indeed the trend in Table 2. Therefore, it is preferable to use only nuclei with short half-lives to determine if any renormalization of the β-strength function is needed to reproduce on the average the experimental half-lives. However, for a short half-life cutoff, for example 1 s, there are not enough data points for a reliable determination. Slightly higher half-life cutoffs indicate $M_{r_1}^{10} \approx 1$, except for the e-e case. However, there are only a few data points for the e-e case, so the higher $M_{r_1}^{10}$ obtained in this case may be unreliable, especially in view of the results obtained below for β^+ decay.

In Table 3 we show the results of an evaluation of the quantities in Eq. (26) for β^+ decay and electron capture of nuclei with $T_{\beta,\mathrm{exp}} \leq 1000$ s. Above we argued in the case of β^- decay that as nuclei with longer half-lives are included, one can expect the calculated half-lives to be too long because the rates due to first-forbidden decay are not included. However, we see instead a slightly opposite trend here. But from arguments similar to those used in the discussion of β^- decay we conclude that in β^+ decay our results are consistent with zero average deviation between calculated and experimental half-lives. Thus, the error in the calculation is given by $\sigma_{r_1}^{10}$ only. The behavior of $\sigma_{r_1}^{10}$ as $T_{\beta,\mathrm{exp}}^{\mathrm{max}}$ increases is similar for both β^- and β^+ decay. Just as when the average deviation is determined, one should not consider decays with too-long half-lives when determining $\sigma_{r_1}^{10}$. On the other hand, it would be desirable to base the determination of $\sigma_{r_1}^{10}$ on a large set of data. Both of these conditions cannot be well-fulfilled simultaneously. However, if we base our estimate of the model error $\sigma_{r_1}^{10}$ by weighting most heavily half-lives in the shorter range, we find that the model error is about a factor of four.

Certain additional assumptions and approximations [18]) have been made to extend the odd-A

Table 3: Analysis of the discrepancy between calculated and measured β^+-decay and electron-capture half-lives shown in Fig. 26.

	n	M_{r_1}	$M_{r_1}^{10}$	σ_{r_1}	$\sigma_{r_1}^{10}$	$T_{\beta,\mathrm{exp}}^{\mathrm{max}}$ (s)
o-o	21	0.17	1.49	0.60	3.99	1
o-e	30	0.25	1.79	0.60	3.97	1
e-e	9	0.55	3.52	0.31	2.03	1
o-o	43	0.09	1.22	0.76	5.77	10
o-e	77	0.03	1.07	0.53	3.38	10
e-e	33	0.21	1.62	0.65	4.46	10
o-o	85	0.11	1.30	1.06	11.37	100
o-e	149	−0.14	0.73	0.52	3.33	100
e-e	63	−0.01	0.98	0.55	3.52	100
o-o	146	0.14	1.37	1.24	17.49	1000
o-e	238	−0.20	0.63	0.65	4.47	1000
e-e	101	−0.08	0.83	0.50	3.16	1000

QRPA formalism to the odd-odd case. If these simplifications were inadequate, one would expect to see a larger σ_{r_1} in the o-o case than in the o-e case. No clear effect of this type is seen in Table 3 for the shorter half-lives but does develop for very long experimental half-lives.

We have already mentioned that particle-particle correlations are not taken into account in our QRPA treatment. These correlations are expected to strongly suppress β^+ transitions,[21,39]) and as a consequence lead to longer half-lives than those obtained in a model that does not consider these correlations. However, our results in Figs. 22–27 and Tables 2 and 3 show that in a standard treatment with $\chi_{\rm GT} = 23$ MeV/A and no renormalization coefficient, we obtain β^+-decay rates that actually agree better with experiment than do our calculated β^--decay rates.

3.6 Proton separation energies

One- and two-proton separation energies are shown versus N and Z in Figs. 9–11. For odd Z the region of known nuclei extends into the region where proton emission is energetically allowed in several places, but especially just above $N = 82$. However, the Coulomb barrier severely inhibits proton emission from the ground state when the energy released is small. Proton emission is therefore more readily observed as delayed emission following β decay.[40,41])

The discrepancy between experimental one-proton separation energies obtained from mass differences and calculated one-proton separation energies is shown in Fig. 12. The biggest errors occur near the magic numbers. There is a general decrease of the error as A increases.

3.7 α-decay properties

The calculated energy release and associated half-life with respect to α decay are plotted in Figs. 13 and 14, respectively.

In 1989 Münzenberg *et al.*[42]) compared the α-decay energy release along the $N = 154$ and 155 isotonic lines to predictions of the FRLDM (1988).[43]) In Fig. 28 we make a similar comparison of measured data to predictions of the current FRDM (1992).[1]) These results based on the current FRDM (1992) agree much better with the measured values than do the corresponding results calculated from our older mass model in 1989 by Münzenberg *et al.*,[42]) and also much better than the results obtained with the 1991 version of the FRDM.[44]) The improvement is due partly to the inclusion of the ϵ_6 shape degree of freedom.

From the Table we find that the nucleus ^{272}110 has a calculated α-decay half-life of 71 ms. The nuclei ^{288}110 and ^{290}110 in the center of the superheavy island have calculated α-decay half-lives of 4 y and 1565 y, respectively. With the 1991 version of the FRDM we obtained calculated α-decay half-lives of 16 ms, 161 y, and 438 y for ^{272}110, ^{288}110, and ^{290}110, respectively. Our current results are different from these older ones for two reasons. First, we now use the new mass model FRDM (1992). Second, we now use a new set of constants in Eq. (24). For ^{288}110 the value of Q_α is 7.36 MeV in our current model, but only 6.95 MeV in the FRDM (1991). For ^{272}110 the difference in Q_α values is only 0.04 MeV, and the difference in the calculated half-lives is in this case due almost entirely to the new set of constants used in Eq. (24).

In the introduction to Sec. 3 we pointed out that because the calculated potential-energy surfaces for some very proton-rich nuclei are very flat and contain multiple minima, the ground-state deformation may exhibit large fluctuations between neighboring nuclei. For example, we see in Ref.[1]) that the calculated quadrupole deformation of ^{318}128 is $\epsilon_2 = 0.0$ whereas $\epsilon_2 = 0.392$ is obtained for ^{319}128. Such deformation changes are accompanied by non-smooth changes in calculated energy releases and associated half-lives. An α-decay half-life of $10^{-8.15}$ s is obtained for ^{318}128, whereas the calculated α-decay half-life for ^{319}128 is greater than 10^{20} s. Because of very short spontaneous-fission half-lives for such proton-rich nonspherical nuclei, we do not expect these nuclei to be observable despite their calculated long α-decay half-lives.

4 EXTRAPOLATEABILITY

Theories are often characterized by their rms error with respect to experimental data points. However, this is often unsuitable because the rms error contains contributions from errors in the experimental data points and is therefore always larger than the intrinsic error of the theory. On the other hand, it is possible to determine the intrinsic error of a theory in a way that contains no contributions from experimental errors.[43]) It is most natural to characterize the deviation between measured data points and theoretical calculations by two quantities: (1) the mean deviation $\mu_{\rm th}$ of the theory from the data points and (2) the standard deviation $\sigma_{\rm th}$ of the theoretical results about this mean.[1,45,46]) Alternatively, one may characterize the error of a theory by a single number, the second central moment of the error term of the theory, which we denote by $\sigma_{{\rm th};\mu=0}$. This measure is similar to the rms deviation, but without the deficiency of contributions from experimental errors. We use these four error measures in our discussions of model accuracies below.

After we completed our mass model,[1]) a new compilation of experimental ground-state masses[3,4]) has become available. We are therefore now able to compare our FRDM (1992) predictions to data that were not taken into account when the model constants were determined, instead of studying the model reliability through simulation. In Table 4 we give errors for the FRDM(1992) for ground-state masses and six separation energies and energy releases for both the region in which the model constants were determined and in the new region of nuclei.

We see in Table 4 that the error $\sigma_{{\rm th};\mu=0}$ for new masses, 0.642 MeV, is 4% *smaller* than the error 0.669 MeV in the region where the model constants were determined. Thus, we conclude, as was done in our mass paper[1]) through simulations, that the model is very well-behaved as one moves away from stability to new regions of nuclei. Indeed, at this stage there is no sign that the model diverges. *It is also very clear that it is not possible to use the rms deviation as a proper measure of model error.* It is 7% larger in the new region of nuclei, although we have just shown that the true model error is actually 4% smaller in the new region of nuclei than in the region where the model constants were determined. This is because the experimental errors in the new region of nuclei are quite large and contribute significantly to the rms error, whereas they are normally quite small in the region of previously known nuclei.

In the absence of correlations in the model error between neighboring masses, the model error for the separation energies and energy releases would be $\sqrt{2}$ times the mass error. However,

Table 4: Theoretical errors and extrapolateability of the FRDM (1992).

	Original nuclei (1989)			New nuclei (1989–1993)				
	$N_{\rm nuc}$	$\sigma_{{\rm th};\mu=0}$ (MeV)	rms (MeV)	$N_{\rm nuc}$	$\mu_{\rm th}$ (MeV)	$\sigma_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	rms (MeV)
$M_{\rm th}$	1654	0.669	0.681	217	0.074	0.638	0.642	0.730
$S_{\rm 1n}$	1464	0.393	0.411	195	0.033	0.525	0.526	0.624
$S_{\rm 2n}$	1403	0.539	0.555	198	0.026	0.575	0.576	0.684
Q_{β^-}	1353	0.488	0.507	216	0.006	0.559	0.559	0.647
$S_{\rm 1p}$	1400	0.381	0.397	210	0.068	0.576	0.581	0.672
$S_{\rm 2p}$	1314	0.493	0.509	193	0.026	0.585	0.586	0.663
Q_α	1450	0.625	0.641	224	0.021	0.675	0.675	0.772

Table 5: Comparison of theoretical errors and extrapolateability of the FRDM (1992) with those of the ETFSI-1 (1992) model.

	Original nuclei (1989)					New nuclei (1989–1993)					
		FRDM		ETFSI-1			FRDM			ETFSI-1	
	$N_{\rm nuc}$	$\sigma_{{\rm th};\mu=0}$ (MeV)	rms (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	rms (MeV)	$N_{\rm nuc}$	$\mu_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	rms (MeV)	$\mu_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	rms (MeV)
$M_{\rm th}$	1540	0.607	0.615	0.733	0.742	213	0.070	0.645	0.716	0.015	0.809	0.866
$S_{\rm 1n}$	1356	0.335	0.346	0.514	0.521	190	0.033	0.525	0.609	0.044	0.612	0.681
$S_{\rm 2n}$	1301	0.477	0.482	0.501	0.508	192	0.028	0.580	0.659	−0.052	0.576	0.659
Q_{β^-}	1259	0.425	0.436	0.679	0.684	212	0.001	0.560	0.646	−0.003	0.741	0.791
$S_{\rm 1p}$	1296	0.324	0.339	0.466	0.472	205	0.073	0.581	0.660	0.113	0.608	0.709
$S_{\rm 2p}$	1217	0.434	0.444	0.520	0.531	189	0.030	0.589	0.662	0.082	0.586	0.674
Q_{α}	1342	0.541	0.546	0.520	0.529	217	0.018	0.670	0.762	0.004	0.618	0.699

Table 4 shows that the separation-energy and energy-release errors are instead somewhat *smaller* than the mass-model error. This is due to the correlation in the mass-model error for neighboring nuclei. The separation-energy and energy-release errors increase in the new region of nuclei, whereas the mass-model error does not. This indicates that the correlation between mass-model errors for neighboring nuclei decreases in the new region. Since a mass model should not be judged on the amount of error correlations between nearby nuclei, one cannot gain significant insight about a model by comparing the error of the separation energies and energy releases in the region where the model constants were determined to the errors in a new region of nuclei. However, because many of these quantities are used in astrophysical calculations, there is a practical need to know the errors of these quantities, and it is for this purpose that we provide them.

In Table 5 we compare the errors of the FRDM (1992) and the 1992 extended Thomas-Fermi Strutinsky-integral model (version 1) of Aboussir, Pearson, Dutta, and Tondeur [47,48]) in the region of nuclei where the ETFSI-1 (1992) model constants were determined and in the region of new nuclei that are included in the ETFSI-1 (1992) calculation. The region of nuclei considered in the ETFSI-1 (1992) model is slightly different from the region considered in the FRDM (1992). Its constants were also determined from an adjustment to a slightly earlier mass evaluation. [49]) In Table 5 the quantities pertaining to the FRDM (1992) are also evaluated for this more limited region. Therefore, the results for the FRDM (1992) in Table 5 are slightly different from those in Table 4. The finalized ETFSI-1 (1992) mass table, as it appears in Ref. [48]), differs slightly from an earlier table circulated privately before publication. We use here the finalized, published version.

The comparison in Table 5 between the extrapolateability of the FRDM (1992) and the ETFSI-1 (1992) model shows that for these particular regions the FRDM (1992) error increases by 6% and the ETFSI-1 (1992) model error increases by 10% in the new region relative to the region where the ETFSI-1 (1992) model constants were determined. Thus, we conclude from Tables 4 and 5 that the FRDM (1992) is somewhat more stable as one moves away from stability than is the ETFSI-1 (1992) model.

In Table 6 we compare the extrapolateability between the FRDM (1992/1977) and the 1976

Table 6: Comparison of theoretical errors and extrapolateability of the FRDM (1992/1977) with those of the mass formula of von Groote *et al.* (1976).

	Original nuclei (1977)			New nuclei (1977–1989)					New nuclei (1989–1993)				
		FRDM	v. Groote		FRDM		v. Groote			FRDM		v. Groote	
	$N_{\rm nuc}$	$\sigma_{{\rm th};\mu=0}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	$N_{\rm nuc}$	$\mu_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	$\mu_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	$N_{\rm nuc}$	$\mu_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)	$\mu_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)
$M_{\rm th}$	1323	0.671	0.629	351	0.004	0.686	0.612	1.154	217	0.030	0.668	0.808	1.284
$S_{1{\rm n}}$	1139	0.391	0.383	335	−0.032	0.406	−0.107	0.431	195	0.024	0.525	−0.095	0.541
$S_{2{\rm n}}$	1092	0.508	0.480	320	−0.053	0.632	−0.171	0.650	198	0.007	0.576	−0.213	0.609
Q_{β^-}	1052	0.467	0.516	314	0.077	0.552	0.193	0.737	216	0.031	0.562	0.178	0.633
$S_{1{\rm p}}$	1105	0.361	0.412	305	0.039	0.463	0.102	0.548	210	0.083	0.585	0.157	0.619
$S_{2{\rm p}}$	994	0.478	0.501	331	0.049	0.546	0.160	0.691	193	0.056	0.591	0.217	0.738
Q_α	1144	0.627	0.525	321	−0.005	0.630	−0.001	0.669	224	0.011	0.675	0.024	0.674

mass formula of von Groote, Hilf, and Takahashi.[50]) In this comparison we have adjusted the constants of the FRDM to similar masses[51]) as those considered by von Groote *et al.* in the determination of their constants. Clearly, the mass formula of von Groote *et al.* diverges severely in new regions of nuclei.

In Figs. 29–37 we plot the deviations between calculated and experimental masses, one-neutron separation energies, and energy releases for β^- decay for these three models. Tables 4–6 and Figs. 35–37 are based on *all* Q_{β^-} values, both positive and negative. Neither the FRDM (1992) nor the ETFSI-1 (1992) model shows large divergences in the new region, but strong systematic deviations occur in the model of von Groote *et al.*

We have also made a limited study of the extrapolateability of the recent 1994 Thomas-Fermi model of Myers and Swiatecki.[52,53]) In this model, the macroscopic energy is calculated for a generalized Seyler-Blanchard nucleon-nucleon interaction by use of the original Thomas-Fermi approximation. For $N, Z \geq 30$ the shell and pairing corrections were taken from the 1992 finite-range droplet model, and for $N, Z \leq 29$ a semi-empirical expression was used. The constants of the model were determined by an adjustment to the ground-state masses of the same 1654 nuclei with $N, Z \geq 8$ ranging from ^{16}O to ^{263}106 whose masses were known experimentally in 1989 that were used in the 1992 finite-range droplet model. The theoretical error corresponding to these 1654 nuclei is 0.640 MeV. The reduced theoretical error relative to that in the 1992 finite-range droplet model arises primarily from the use of semi-empirical microscopic corrections in the region $N, Z \leq 29$ rather than microscopic corrections calculated more fundamentally. The theoretical error for 217 newly measured masses is 0.737 MeV, corresponding to an increase of 15%. This model therefore extrapolates to new regions somewhat less well than does either the FRDM (1992) or the ETFSI-1 (1992) model. The deviations between experimental and calculated masses for these 217 new nuclei are shown in Fig. 38.

In the Wapstra-Audi mass evaluations[2–4,49]) there usually are listed not only measured masses, but also masses estimated from systematic trends. It is unfortunate that some theoretical mass studies have not observed the difference between measured masses and masses given by systematic trends, and included also the latter in the data set to which the model parameters were adjusted. The masses given by systematic trends have to be considered on the same basis as masses given by other models. We may therefore study the reliability of the Wapstra-Audi

systematic-trend model by use of the methods applied above to other models. We consider the masses given by systematic trends in the 1989 midstream evaluation [2]) as model masses and compare them to the new masses determined in the 1993 mass evaluation. [3,4]) The result is shown in Fig. 39. The systematic-trend model error in the new region is 0.404 MeV, which is smaller than the error of the FRDM (1992). However, the systematic-trend model does not provide masses very far from known nuclei, and indeed many of the newly measured masses were not predicted by the 1989 systematic-trend model. Also, in this case it is not possible to provide a ratio between the error for nuclei in the new region and the error in the known region.

The discovery in late 1994 of the new element $Z = 111$ [30]) allows us to test model extrapolateabilities in the region of large proton numbers. In Fig. 40 we compare the experimental results for the α-decay chain of the heaviest known element $^{272}111$ with predictions obtained in the FRDM (1992), the ETFSI-1 (1992) model [47,48]), and the 1992 fermion dynamical symmetry model of Han, Wu, Feng, and Guidry. [54]) Clearly the predictions of the FRDM (1992) agree much better with the new experimental data than do those of the other two models. The FRDM (1992) error for this chain is in fact considerably smaller than the error in the region where the model constants were adjusted, whereas the errors for the other two models, especially the FDSM (1992), are considerably larger than in the regions where the constants of these two models were adjusted. Because the FRDM (1992) Q_α error is about 0.5 MeV for heavy nuclei in the known region, one should not consistently expect the exceptionally good agreement present in Fig. 40 for all new α-decay chains that are discovered in the heavy region. However, the agreement between experiment and predictions of the FRDM (1992) seen in this figure, plus better-than-expected agreement between experiment and predictions of the FRDM (1992) and the decay chains of another recently discovered element with proton number $Z = 110$, [29]) confirm the conclusion reached earlier by simulation [1]) that the FRDM (1992) is reliable to its stated accuracy as we move away from the region of known elements towards the superheavy region.

5 ASTROPHYSICAL APPLICATIONS

Nuclear physics and astrophysics share several common themes: (1) the nuclear reactions that are responsible for nucleosynthesis and isotopic abundance patterns in nature, (2) the energy sources of stellar events via static or explosive nuclear burning, and (3) the behavior of nuclear matter at and beyond nuclear densities, including the equation of state for type-II supernova (SN II) explosions and neutron stars.

Here, we focus on explosive conditions in which large numbers of free protons or neutrons are available. They can lead to the synthesis of nuclei far from stability either via rapid proton capture and β^+ decay (rp-process) in novae and X-ray bursts or rapid neutron capture and β^- decay (r-process) in SN II. In both cases, theoretical studies require reaction rates and other nuclear properties of unstable nuclei which, to a large extent, are not known experimentally. Hence, a general understanding of their nuclear-structure properties can be obtained only through theoretical means.

Because several different nuclear quantities are needed in rp- and r-process calculations, in the past it was not possible to obtain them all from one source. Taking them from different sources, however, raises questions of consistency. In such mixed-model calculations, [55]) although often performed due to the lack of a unified approach, occasionally nuclear structure signatures may vanish or artificial effects may occur, thus strongly limiting their predictive power far from stability. Therefore, attempts to use this approach to identify the sites of rp- and r-processes may lead to erroneous conclusions. Consequently, it is of great importance to provide nuclear-structure properties based on a single, unified theoretical framework within which all quantities of interest can be obtained. We illustrate this principle below with an example.

5.1 The *rp*-process

In a recent paper van Wormer *et al.*[56]) have evaluated in detail the nuclear-reaction sequences for conditions in explosive hydrogen burning at temperatures beyond 10^8 K, corresponding to the *rp*-process, a sequence of rapid proton-capture reactions and β^+ decays passing through proton-rich nuclei. Such processes typically occur when hydrogen fuel is ignited under highly degenerate conditions in explosive events on the surface of compact objects like white dwarfs (novae) and neutron stars (*X*-ray bursts). Hydrogen burning at high temperatures such as 2×10^9 K may also occur in a stable fashion in so-called Thorne-Zytkow objects. Such objects are expected to result from the merging of a neutron star and a main-sequence star in a binary system. An *rp*-process occurs then at the base of a fully convective envelope just above the neutron core, giving the object the appearance of a red supergiant.

As pointed out by some authors,[56,57]) the *rp*-process cannot be explained in a simple and clean fashion in terms of a (p,γ) $\rightleftharpoons$ (γ,p) equilibrium in all isotopic chains. Under such circumstances, the nuclear data needed for a theoretical description would be limited to nuclear masses and corresponding proton separation energies and β^+-decay half-lives. However, the Coulomb barriers in charged-particle captures lead to a cycle pattern with capture and decay time scales of similar size. As outlined in Fig. 41, the *rp*-process at low temperatures is dominated by two successive proton captures, starting out from an e-e nucleus, a β^+ decay, a further proton capture into an even-Z nucleus, another β^+ decay, and a final (p,α) reaction close to stability.

The progress of the *rp*-process towards heavier nuclei depends on the leakage ratio (p,γ)/(p,α) into the next cycle. Increasing temperature makes it possible to overcome Coulomb barriers and extend the cycles to more proton-rich nuclei, which permits additional leakage via proton captures competing with long β decays. Beyond 3×10^8 K, all cycles break open and a complete *rp*-pattern of proton captures and β decays is established, which may reach beyond ^{56}Ni.[56,57])

As a consequence, along with the separation energies and half-lives that are required for an equilibrium assumption, proton and α-capture rates for unstable nuclei are also required as nuclear-physics input into the reaction network. In current calculations the majority of these reaction rates are not based on measured cross sections, but are usually approximated by simple statistical-model calculations.[58]) Even such statistical approaches require a number of input quantities, such as (1) ground-state spins and parities of target, compound, and final nuclei, (2) reaction energy releases, (3) realistic nucleon-nucleus and α-nucleus optical potentials, (4) giant-dipole resonance energies and widths, and (5) level-density models. It is desirable to improve the accuracy of current level-density models by utilizing shell and pairing corrections of modern mass models.

5.2 The *r*-process

The *r*-process was inferred[59,60]) from the observation of characteristic peaks in the abundance curve of β-stable nuclei. The peak maxima are located 4, 4, and 9 neutrons *below* the magic neutron numbers 50, 82, and 126, respectively. In Fig. 16 some basic features of the *r*-process are outlined. The position of the *r*-process line depends on nuclear-structure properties and the stellar conditions under which it occurs, in particular the temperature, density, and duration of the neutron flux. The line plotted in the figure corresponds to a neutron separation energy of 2.4 MeV. The *r*-process is dynamic and may be located anywhere in the region 1.5 MeV $< S_{1n} <$ 3.0 MeV, depending on the stellar conditions. Magic neutron numbers play a special role in the *r*-process as is partially seen in Fig. 16, where the *r*-process line has a kink at each magic neutron number. In addition, nuclei pile up at these magic neutron numbers because of the long β-decay half-lives and sudden lowering of the neutron-capture cross section that occurs at magic neutron numbers. After freezeout of the neutron flux, these nuclei β decay back towards the line of β stability. It is easy to see from the figure that the peaks in the abundance

curve are related to a concentration of neutron-magic nuclei *far from β stability*. In fact, this effect has been used to put rough constraints on nuclear masses far from β stability and to rule out nuclear mass models with predictions far from these constraints. The decay back to the line of β stability is also influenced by β-delayed neutron emission.

Since the pioneering work of Burbridge *et al.*[59]) and Cameron[60]) the rapid neutron capture process has been associated with explosive environments with high temperature $T \geq 10^9$ K and high neutron-number density $n_{\rm n} \geq 10^{20}$ cm^{-3}. Under such conditions, the neutron-capture time scales of heavy nuclei are so short that within about 10^{-4} s highly neutron-rich nuclei can be produced up to 15 to 30 mass units away from β stability with neutron separation energies $S_{1\rm n} \approx 1.5$ to 3.0 MeV. Neutron captures are not hindered by increasing Coulomb barriers, in contrast to the case for the *rp*-process in the previous section. Magic neutron numbers are encountered for smaller mass numbers A than in the valley of stability, which, after freezeout and β decay, shifts the observed solar-system *r*-process abundance peaks below the *s*-process peaks. However, besides this basic understanding, the history of *r*-process research has been quite diverse in suggested astrophysical scenarios, as well as with the required size of the nuclear network.[55])

The observed isotopic *r*-abundances $N_{r,\odot}$ shown in Fig. 16 are the result of successive neutron captures along the *r*-process path and β^- decay back to stability, thus depending, apart from stellar parameters, on a variety of nuclear properties of nuclei with extreme N/Z ratios. In the general case, among nuclear-physics quantities, ground-state masses and corresponding Q_β values, neutron-separation energies $S_{1\rm n}$, β^--decay half-lives, probabilities of β-delayed neutron emission $P_{\rm n}$, neutron-capture cross sections, and ground-state spins and deformations are of importance in *r*-process calculations.[55,61]) For the first time, most of these quantities can be obtained from a single, unified model, namely our present macroscopic-microscopic model. Neutron-capture rates are so far calculated with the statistical Hauser-Feshbach model, as long as the level density in the compound nucleus is sufficiently high to justify such an approach. As is the case for proton captures discussed in Sec. 5.1, this method requires a knowledge of additional quantities, such as optical potentials and giant-dipole-resonance and level-density parameters. For nuclei in the *r*-process path, in particular near closed neutron shells, the level density is small and the Hauser-Feshbach approach might no longer be applicable. In these cases, Breit-Wigner resonance capture and direct capture have to be considered, again requiring additional nuclear-physics properties as input for the respective model calculations.[61,62]) For nuclei with $Z \geq 80$, fission barriers and rates of β-delayed as well as neutron-induced fission are also important. Finally, within the recently favored "hot-entropy-bubble" *r*-process scenario,[63,64]) charged-particle reactions during the so-called α-rich freezeout are also required in the $A \approx 80$ region. Taken together, all these nuclear data for thousands of mostly unknown isotopes require a huge reaction network for "complete" *r*-process calculations.

Primarily in order to facilitate these complicated and time-consuming calculations, since 1957 many attempts to predict the $N_{r,\odot}$ distribution were based on the simplified assumption of the (n,γ) $\rightleftharpoons$ (γ,n) equilibrium concept.[55,59,61]) When assuming in addition a steady-flow equilibrium of β decays, the prediction of *r*-abundances requires only the input of nuclear masses and corresponding neutron separation energies $S_{1\rm n}$, β-decay half-lives T_β and β-delayed neutron-emission probabilities $P_{\rm n}$, as well as the stellar parameters T_9, $n_{\rm n}$, and the process duration. Whereas for a given $n_{\rm n}$ the $S_{1\rm n}$ determine the *r*-process path, the T_β of the isotopes along this flow path determine, in principle, the progenitor abundances and, when $P_{\rm n}$ branching during freezeout is considered, also the final *r*-abundances. Only in recent years could the validity of this "waiting-point" approximation in combination with a steady β-decay flow be confirmed locally for the $A \approx 80$ and 130 $N_{r,\odot}$ peaks on the basis of the first experimental information in the *r*-process path.[65]) These recent results showed clearly, for example, how the long T_β of the classical $N = 82$ waiting-point nucleus ^{130}Cd directly correlated with the large $N_{r,\odot}$ value of its

isobar ^{130}Te in the $A \approx 130$ abundance peak seen in Fig. 16.

Since there is not yet complete consensus on the stellar site of the r-process and the specific astrophysical conditions under which it takes place, one deductive approach to theoretical r-process studies has been to take the $N_{r,\odot}$ observables [66]) as a constraint that allow the derivation of the necessary conditions required to reproduce these features. Using the unified nuclear-physics basis presented in this paper, supplemented by all experimental data available up to 1991 as well as local improvements of the QRPA calculations, Kratz *et al.* [61]) have obtained significant progress in reproducing the $N_{r,\odot}$ pattern relative to the situation five or ten years ago. As an example, we show in Fig. 42 results of r-process calculations for two different mass models. The top calculation is based on our 1991 version of the FRDM. [45,67]) Our current FRDM (1992) shown in Fig. 19 has smaller mass and S_{1n} errors, but our preliminary r-process studies with it do not show significantly improved agreement. In the lower part of Fig. 42, nuclear masses and input for the QRPA calculations were taken from the ETFSI-1 (1992) model in its preliminary, privately circulated version.

With the current agreement between $N_{r,\odot}$ data and the calculations, the theoretical treatment is sufficiently accurate that some conclusions can be drawn about the stellar conditions responsible for the production of r-process nuclei. For example, one has found that it is not possible to reproduce the $N_{r,\odot}$ curve assuming a global steady-flow process. Instead, a minimum of three r-components with different neutron densities is required. Each of the components proceeds up to one of the abundance peaks and reaches a local steady-flow equilibrium which breaks down at the top of each peak, situated at one of the $N = 50$, 82, and 126 magic shells. With these results, the explosive He-burning scenarios favored in the 1980s can definitely be ruled out as possible sites for the r-process.

The large deviations from the $N_{r,\odot}$ pattern evident in Fig. 42, especially those just before the abundance peaks at $A \approx 130$ and 195, were interpreted [57,68,69]) as arising from overly strong magic-neutron shell corrections as one moves away from a doubly magic configuration, from the neglect of the proton-neutron residual interaction, and from correlated problems with describing shape transitions in the neutron mid-shell regions around $N = 66$ and 104.

Rather than representing a failure of the FRDM (1992) far from stability, these difficulties are due to normal inaccuracies that occur anywhere in the chart of the nuclides, both near stability and far from stability. They must be expected and considered normal in a model based on such a simple effective interaction as the one-body single-particle potential with a simple pairing residual interaction. Despite some deficiencies, the current models, when used appropriately, have been *sufficiently accurate* to *considerably advance* our understanding of several astrophysical processes and to *identify* specific nuclear-structure features of nuclei far from stability near magic shells and close to the neutron drip lines. These nuclei are normally inaccessible to experiment, but unique signatures of their nuclear structure are well preserved as differences in the observed $N_{r,\odot}$ pattern relative to the pattern calculated with the FRDM (1992). Our identification of specific nuclear-structure features in nuclei far from stability has generated substantial interest in the nuclear-physics community and stimulated several calculations of nuclear masses in limited regions far from stability in terms of self-consistent mean-field theories. [70–72]) Some of these local calculations now produce nuclear masses that remove some of the discrepancies that are present in Fig. 42.

However, to be considered an improvement over current global nuclear-structure calculations, a new theory must achieve more than just a better local description of features that were postulated on the basis of existing theories. To justify the designation new and improved, a new theory should globally reproduce better nuclear masses and other ground-state nuclear-structure effects than does the FRDM (1992). It should achieve these results with a simple, global choice of constants. And, it should, just as has the current FRDM (1992), correctly predict new nuclear-structure features far from stability and serve to further enhance our understanding of

several astrophysical processes. The results achieved so far in new mean-field calculations are important preliminary steps in this direction.

We have seen that certain differences in the abundance fits and remaining deficiencies can be attributed to the nuclear mass models applied. We now want to check whether effects from different half-life sets can also be separated out in our $N_{r,\odot}$ calculations.

As we have discussed earlier,[61]) once the r-process path is defined by a contour line of constant S_{1n} values, the abundances of isotopes in this path are directly related to their β-decay half-lives according to the waiting-point concept.[59]) These β-decay half-lives are determined by the energy window Q_β, on the one hand, and by the low-lying nuclear structures in the Gamow-Teller strength function, on the other hand. As has been discussed in detail elsewhere,[61]) T_β is predominantly influenced by the latter properties. Therefore, statistical models such as the gross theory of β decay,[73]) which neglect nuclear structures, will not be able to describe the β-decay quantities far from stability in an adequate way. It has been well known for more than a decade that, due to the missing nuclear-structure effects, the β-decay half-lives from this model are systematically too long by factors of five to 10 far from stability. Nevertheless, because the gross-theory predictions are still occasionally used in astrophysical calculations,[64,74]) we have for the purpose of illustrating its deficiencies performed some T_β and P_n calculations with this model using Q_β values from both the FRDM (1992) and ETFSI-1 (1992) model. We can show that the differences in the Q_β predictions of the two models for isotopes in the regions of the r-process path affect the T_β values obtained in the gross theory only to a small extent. Therefore the T_β effects in the calculated r-abundances originate mainly from the missing nuclear structures in the β-strength functions of the gross theory.

In Fig. 43 we present a comparison of r-process calculations based on the gross theory and on the QRPA. The upper part of Fig. 43 shows that for our best-fit conditions of the third component,[61]) a switch from the T_β(QRPA) consistent with the FRDM masses to T_β(g.t.) creates r-overabundances in the range $150 \leq A \leq 180$. It is possible to adjust for this artificial effect by a change of astrophysical conditions, for example, by increasing n_n in order to obtain a more neutron-rich r-process path and shorter T_β(g.t.) in that mass region.[74]) However, as can be seen in the lower left-hand part of Fig. 43, higher neutron densities, which improve the $N_{r,\odot}$ fits in the $150 \leq A \leq 180$ range, but are difficult to obtain in realistic r-process scenarios,[63,64]) shift the structure of the $A \approx 195$ peak too far to lower masses and make such an approach invalid. We can only conclude that far from β stability the values of T_β(g.t.) are, in fact, too long.

6 SINGLE-PARTICLE LEVELS

As a final result we present in Figs. 44–99 calculated proton and neutron single-particle level diagrams for representative spherical and deformed nuclei throughout the periodic system. The diagrams are useful for obtaining the spin and parity of low-lying states of odd-even nuclei and for identifying gaps in the level spectra that may be associated with particularly stable proton-neutron combinations.

For heavier nuclei higher-multipole deformations become increasingly important, as can be seen in the mass table and color overview figures in our mass calculations.[1]). For prolate shapes we have therefore chosen ϵ_4 and ϵ_6 to be functions of ϵ_2. The hexadecapole deformation ϵ_4 is either a linear function of ϵ_2 in the entire range $0 \leq \epsilon_2 \leq 0.4$ or linear in the range $0 \leq \epsilon_2 \leq 0.2$ and constant in the range $\epsilon_2 \geq 0.2$, as indicated on the upper horizontal axis. The hexacontratetrapole deformation ϵ_6 is zero when it is not explicitly mentioned in the figure captions. Otherwise, it varies linearly in the entire range $0 \leq \epsilon_2 \leq 0.4$ in the manner indicated in the figure captions.

One notes that proton number $Z = 14$ and neutron number $N = 14$ correspond to well-

developed spherical gaps for several of the lighter systems. The effect of the higher-multipole deformation parameters ϵ_4 and ϵ_6 is clearly visible in the level-diagram sequences shown in Figs. 58–63 and 88–93, for example.

In the heavy region it is particularly interesting that the deformed shell gaps at proton numbers $Z = 104$–110 and neutron number $N = 162$ emerge only for relatively large positive values of the hexadecapole deformation parameter ϵ_4. These gaps give rise to unusual stability, which has made possible the discovery of several new elements in this region.[26–30])

Figure 97 shows the predicted large spherical neutron gap $N = 184$. However, the unusually large density of single-particle levels just above has the consequence that the largest negative microscopic correction occurs approximately at neutron number $N = 178$ in our model.

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Figure captions

Fig. 1 Global microscopic pairing gap for protons. The single-particle levels entering the pairing calculation correspond to ground-state shapes that have been determined by minimizing the total potential energy with respect to ϵ_2, ϵ_4, ϵ_3, and ϵ_6 shape degrees of freedom. The jagged black lines indicate regions where experimental proton pairing gaps may be extracted from fourth-order odd-even mass differences. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines. In the Lipkin-Nogami model it is the sum $\Delta_{\rm p}+\lambda_{2\rm p}$ plotted here that should be compared to odd-even mass differences. In contrast to the behavior of BCS solutions, this sum shows no sign of collapse at magic proton numbers.

Fig. 2 Global microscopic pairing gap for neutrons. The single-particle levels entering the pairing calculation correspond to ground-state shapes that have been determined by minimizing the total potential energy with respect to ϵ_2, ϵ_4, ϵ_3, and ϵ_6 shape degrees of freedom. The jagged black lines indicate regions where experimental neutron pairing gaps may be extracted from fourth-order odd-even mass differences. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines. In the Lipkin-Nogami model it is the sum $\Delta_{\rm n}+\lambda_{2\rm n}$ plotted here that should be compared to odd-even mass differences. In contrast to the behavior of BCS solutions, this sum shows no sign of collapse at magic neutron numbers.

Fig. 3 Discrepancy between experimental proton pairing gaps determined from fourth-order odd-even mass differences and microscopic pairing gaps $\Delta_{\rm LN_p}=\Delta_{\rm p}+\lambda_{2\rm p}$ obtained in the Lipkin-Nogami model. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines. Fairly large discrepancies occur in several places. However, these discrepancies do not necessarily mean that the calculated gaps are incorrect. Instead, it may be that the pairing gap is not determined properly from odd-even mass differences, as discussed in the text. In particular, when large errors in this figure occur in the same region where large errors occur in Fig. 4, sudden shape transitions are probably responsible.

Fig. 4 Discrepancy between experimental neutron pairing gaps determined from fourth-order odd-even mass differences and microscopic pairing gaps $\Delta_{\rm LN_n}=\Delta_{\rm n}+\lambda_{2\rm n}$ obtained in the Lipkin-Nogami model. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines. Fairly large discrepancies occur in several places. However, these discrepancies do not necessarily mean that the calculated gaps are incorrect. Instead, it may be that the pairing gap is not determined properly from odd-even mass differences, as discussed in the text. In particular, when large errors in this figure occur in the same region where large errors occur in Fig. 3, sudden shape transitions are probably responsible.

Fig. 5 Neutron separation energy for odd-neutron nuclei. Each odd-neutron nucleus is represented by a color field *one* unit high and *two* units wide. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei is enclosed by a jagged black line, and magic proton and neutron numbers are indicated by pairs of thin, parallel lines. The region of the nuclear chart where the r-process occurs is approximately 2.0 MeV $< S_{1\rm n} <$ 3.0 MeV for odd N, which in this figure appears in light blue. Recent experiments have reached the r-process region at both $N = 50$ and $N = 82$.

Fig. 6 Neutron separation energy for even-neutron nuclei. Each even-neutron nucleus is represented by a color field *one* unit high and *two* units wide. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei is enclosed by a jagged black line, and magic proton and neutron numbers are indicated by pairs of thin, parallel lines.

Fig. 7 Two-neutron separation energy for odd- and even-neutron nuclei. Each nucleus is represented by a color field one unit high and one unit wide. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei is enclosed by a jagged black line, and magic proton and neutron numbers are indicated by pairs of thin, parallel lines.

Fig. 8 Discrepancy between experimental and calculated one-neutron separation energies. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines. Large discrepancies occur where there are large changes in the mass error between neighboring nuclei, namely at magic numbers and in the light region of nuclei. In the deformed rare-earth and actinide regions the discrepancy is very small.

Fig. 9 Proton separation energy for odd-proton nuclei. Each odd-proton nucleus is represented by a color field *one* unit wide and *two* units high. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei, which is enclosed by a jagged black line, extends in several places to where proton emission is energetically allowed from odd-proton nuclei. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines.

Fig. 10 Proton separation energy for even-proton nuclei. Each even-proton nucleus is represented by a color field *one* unit wide and *two* units high. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei, which is enclosed by a jagged black line, nowhere extends to where proton emission is energetically allowed from even-proton nuclei. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines.

Fig. 11 Two-proton separation energy for odd- and even-proton nuclei. Each nucleus is represented by a color field one unit wide and one unit high. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei, which is enclosed by a jagged black line, barely extends to where two-proton emission is energetically allowed. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines.

Fig. 12 Discrepancy between experimental and calculated one-proton separation energies. Magic proton and neutron numbers are indicated by pairs of thin, parallel lines. Large discrepancies occur where there are large changes in the mass error between neighboring nuclei, namely at magic numbers and in the light region of nuclei. In the deformed rare-earth and actinide regions the discrepancy is very small.

Fig. 13 Energy released in α decay. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei is enclosed by a jagged black line, and magic proton and neutron numbers are indicated by pairs of thin, parallel lines. The calculations show that Q_α is in the range 6–9 MeV in the heaviest known region and 9–12 MeV in the deformed superheavy island surrounding $^{272}110$.

Fig. 14 Global α-decay half-life calculated from a semi-empirical relationship between T_α and Q_α. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei is enclosed by a jagged black line, and magic proton and neutron numbers are indicated by pairs of thin, parallel lines.

Fig. 15 Global microscopic β-decay half-life for allowed Gamow-Teller transitions. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The region of known nuclei is enclosed by a jagged black line, and magic proton and neutron numbers are indicated by pairs of thin, parallel lines. Above the black squares the calculated combined half-life with respect to β^+ decay and electron capture is plotted; below the black squares the half-life with respect to β^- decay is plotted.

Fig. 16 Features of the r-process. Black squares denote β-stable nuclei. Where available, experimental masses were used to determine the location of β-stable nuclei; otherwise, calculated masses were used. The colored region in the main graph shows calculated half-life with respect to β^- decay. The jagged black line gives the right-hand boundary of the region of known nuclei. The thick magenta line represents $S_{1n} = 2.4$ MeV, which is the approximate location of the r-process path for a particular set of stellar conditions. The magenta squares in the region of β-stable nuclei are created in decay from the r-process line. The solar r-process abundance shown in the insert is plotted versus the mass number A, whose axis is curved slightly to follow the line of β-stability. A line perpendicular to the valley of β-stability and originating at a particular mass value crosses the A axis of the insert plot at right angles at this value and also passes through the circle giving the abundance for this A value.

Fig. 17 Comparison of calculated and experimental nuclear ground-state spins and parities for odd-even nuclei in the light and medium-mass regions. Spherical assignments are used in the calculations when $|\epsilon_2| < 0.15$. Many of the discrepancies occur in transition regions between spherical and deformed nuclei or where several levels are grouped close together.

Fig. 18 Similar to Fig. 17 but for the heavy region. The discrepancies in the heaviest part of the actinide region occur because here several neutron single-particle levels are grouped very close together.

Fig. 19 Comparison of experimental and calculated microscopic corrections for 1654 nuclei in the 1992 version of the finite-range droplet model.[1,46]) The bottom part showing the difference between these two quantities is equivalent to the difference

between measured and calculated ground-state masses. There are almost no systematic errors remaining for nuclei with $N \geq 65$, for which region the theoretical error is only 0.448 MeV.

Fig. 20 Calculated Gamow-Teller β-strength function for ^{95}Rb. Whereas for the calculation of the quantities in the Table we use the shapes obtained in our mass calculation, [1]) in this figure we use the spherical shape because we wish to show a typical spherical β-strength function and because experimentally ^{95}Rb is spherical. The arrows with wide heads denote successive neutron-separation energies in the daughter, and the arrow with a thin head denotes the value of Q_β. The calculated strength containing only a few large peaks in the low-energy region is typical of a spherical nucleus. Since all the strength is calculated to be above the one-neutron separation energy, the theoretical probability P_n for β-delayed neutron emission is 100%. Experimentally, there is a large peak in the GT strength function in the region 3.5–4.0 MeV, so experimentally the β-delayed neutron emission probability is only 8.5%.

Fig. 21 Calculated Gamow-Teller β-strength function for ^{99}Rb. Here we use the shape obtained in our mass calculation. The strength function is typical of that of a deformed nucleus. Because there is a higher likelihood of significant strength in the low-energy region for deformed nuclei than for spherical nuclei there is a characteristic, large decrease in the β-decay half-life at the shape transition. Since there is considerable strength below the neutron-emission threshold the β-delayed neutron-emission probability is low.

Fig. 22 Ratios between calculated and experimental half-lives for β^- decay as functions of neutron number N. There are no systematic effects versus N.

Fig. 23 Ratios between calculated and experimental half-lives for β^- decay as functions of the experimental half-life for β^- decay. As expected, we find a very strong correlation between the error and the experimental β-decay half-life. The correlation is such that we can expect fairly reliable half-life calculations far from β-stability, in the region of interest for astrophysical r-process calculations. An analysis of the results in this figure is presented in Table 2 and is also discussed in the text.

Fig. 24 Ratios between calculated and experimental half-lives for β^- decay as functions of Q_β. The discrepancy is expected to be larger for low values of Q_β because the calculated half-life is most sensitive here to errors in the positions of the peaks in the strength functions.

Fig. 25 Ratios between calculated and experimental half-lives for β^+ decay and electron capture as functions of neutron number N. There are no systematic effects versus N.

Fig. 26 Ratios between calculated and experimental half-lives for β^+ decay and electron capture as functions of the experimental half-life for β^+ decay and electron capture. Surprisingly, there is no strong correlation between the error and $T_{\beta,\mathrm{exp}}$, except for odd-odd nuclei. An analysis of the results in this figure is presented in Table 3 and is also discussed in the text.

Fig. 27 Ratios between calculated and experimental half-lives for β^+ decay and electron capture as functions of Q_β. Only the error for odd-odd nuclei is correlated with Q_β.

Fig. 28 Comparison between experimental and calculated energy releases Q_α for the $N = 154$ and 155 isotonic chains. The experimental data are from Fig. 6 of Münzenberg *et al.*,[42]) where the data are compared to predictions of the FRLDM (1988). The new results presented here agree with the data much better. The improvement is due partly to the inclusion of the ϵ_6 shape degree of freedom.

Fig. 29 Calculation to show the reliability of the FRDM (1992) in new regions of nuclei. The FRDM (1992) was adjusted to 1654 masses known in 1989.[2]) The figure shows the deviations between experimental and calculated masses for 217 new nuclei whose masses were measured between 1989 and 1993.[3,4]) The error is 4% *smaller* in the new region compared to that in the region where the model constants were adjusted. There are no systematic effects visible in the figure.

Fig. 30 Calculation to show the reliability of the ETFSI-1 (1992) in new regions of nuclei. The ETFSI-1 (1992) was adjusted to masses known in 1988.[49]) The figure shows the deviations between experimental and calculated masses for 210 new nuclei whose masses were measured between 1989 and 1993.[3,4]) The error is 10% larger in the new region compared to that for the 1989 data set[2]) we have available, which is only marginally different from the 1988 data set to which the model constants were adjusted. There are no systematic effects visible in the figure.

Fig. 31 Similar to Figs. 29 and 30 but for the mass formula of von Groote *et al.*[50]) With its postulated shell corrections and more adjustable constants than in our model with *calculated* shell corrections, the error in the new region is 104% larger than for a 1977 set of measured masses,[51]) which is only marginally different from the set of masses where the constants were adjusted. There is also a systematic increase in the error with increasing distance from β stability.

Fig. 32 Calculation to show the reliability of one-neutron separation energies obtained from the FRDM (1992) in new regions of nuclei. There are no systematic effects visible in the figure.

Fig. 33 Calculation to show the reliability of one-neutron separation energies obtained from the ETFSI-1 (1992) model in new regions of nuclei. There are no systematic effects visible in the figure, apart from an odd-even staggering related to problems in the pairing part of the ETFSI-1 (1992) model.

Fig. 34 Calculation to show the reliability of one-neutron separation energies obtained from the mass formula of von Groote *et al.* in new regions of nuclei. On the neutron-rich side the calculated one-neutron separation energies are systematically too high by 0.29 MeV.

Fig. 35 Calculation to show the reliability of energy releases for β^- decay obtained from the FRDM (1992) in new regions of nuclei. There are no systematic effects visible in the figure.

Fig. 36 Calculation to show the reliability of energy releases for β^- decay obtained from the ETFSI-1 (1992) model in new regions of nuclei.

Fig. 37 Calculation to show the reliability of energy releases for β^- decay obtained from the mass formula of von Groote *et al.* in new regions of nuclei. On the neutron-rich side the calculated energy releases are systematically too low by 0.52 MeV. Corresponding β-decay rates based on these values would be too slow.

Fig. 38 Calculation to show the reliability of the TF (1994) model in new regions of nuclei. The TF (1994) model was adjusted to 1654 masses known in 1989.[2]) The figure shows the deviations between experimental and calculated masses for 217 new nuclei whose masses were measured between 1989 and 1993.[3,4]) The error is 15% larger in the new region compared to that in the region where the model constants were adjusted. There are no systematic effects visible in the figure.

Fig. 39 Calculation to show the reliability of the Wapstra-Audi systematic-trend mass model in new regions of nuclei. The systematic-trend masses were provided in the 1989 midstream mass evaluation.[2]) The figure shows the deviations between experimental and systematic masses for 187 new nuclei that were given by systematic trends in the 1989 evaluation and whose masses were measured between 1989 and 1993.[3,4]) There are no systematic effects visible in the figure.

Fig. 40 Comparison between energy releases Q_α obtained in the FRDM (1992), ETFSI-1 (1992) model, and FDSM (1992) and recent experimental data for the heaviest known element.[30]) When several values of Q_α were measured we choose for the figure the highest value.

Fig. 41 The hot hydrogen burning cycles,[57]) typically consisting of three proton captures, two β^+ decays, and a closing (p,α) reaction. Break-out towards heavier nuclei occurs only via the (p,γ)/(p,α) branching at the cycle closings. Because of the ^{18}F(p,α) reaction no OFNe cycle exists, which would otherwise connect the CNO and NeNaMg cycles.

Fig. 42 Calculated r-process abundances (solid lines) compared to measured values (solid circles). For both the upper and lower parts of the figure β-decay half-lives and delayed-neutron emission probabilities are calculated in a QRPA model based on folded-Yukawa single-particle energies, but experimental information has been used when available. In the upper part of the figure the r-process path was determined from the FRDM (1991),[45,67]) and in the lower part of the figure it was determined from the preliminary, privately circulated version of the ETFSI-1 (1992) model.[47,48])

Fig. 43 Static steady-flow calculations of the r-process abundance $N_{r,\odot}$ for the $135 \leq A \leq 195$ mass region, the so-called "third-component." The right-hand part of the figure shows the best fit obtained with T_β and P_n values from our QRPA model. The upper left-hand part of the figure shows $N_{r,\odot}$ for the same T_9-n_n conditions obtained with the on-the-average five-times longer T_β values from the gross theory.[73]) As can be seen from the lower left-hand part of the figure, with these T_β values reasonable fits for the actinide region require neutron densities of 10^{25} cm^{-3}, which are difficult to obtain in the hot-entropy-bubble r-process scenario.

Fig. 44 Calculated proton single-particle level diagram for nuclei in the vicinity of $^{16}_{8}\mathrm{O}_8$.

Fig. 45 Calculated neutron single-particle level diagram for nuclei in the vicinity of $^{16}_{8}\mathrm{O}_8$.

Fig. 46 Calculated proton single-particle level diagram for proton-rich nuclei in the vicinity of $^{34}_{20}\mathrm{Ca}_{14}$.

Fig. 47 Calculated neutron single-particle level diagram for proton-rich nuclei in the vicinity of $^{34}_{20}\mathrm{Ca}_{14}$.

Fig. 86 Calculated proton single-particle level diagram for nuclei in the vicinity of $^{232}_{90}\mathrm{Th}_{142}$. The hexacontratetrapole deformation ϵ_6 is zero for oblate shapes and is given by $\epsilon_6 = 0.1\epsilon_2$ for prolate shapes.

Fig. 87 Calculated neutron single-particle level diagram for nuclei in the vicinity of $^{232}_{90}\mathrm{Th}_{142}$. The hexacontratetrapole deformation ϵ_6 is zero for oblate shapes and is given by $\epsilon_6 = 0.1\epsilon_2$ for prolate shapes.

Fig. 88 Calculated proton single-particle level diagram for proton-rich nuclei in the vicinity of $^{240}_{100}\mathrm{Fm}_{140}$. The hexacontratetrapole deformation ϵ_6 is zero for oblate shapes and is given by $\epsilon_6 = 0.15\epsilon_2$ for prolate shapes.

Fig. 89 Calculated neutron single-particle level diagram for proton-rich nuclei in the vicinity of $^{240}_{100}\mathrm{Fm}_{140}$. The hexacontratetrapole deformation ϵ_6 is zero for oblate shapes and is given by $\epsilon_6 = 0.15\epsilon_2$ for prolate shapes.

Fig. 90 Calculated proton single-particle level diagram for nuclei in the vicinity of $^{252}_{100}\mathrm{Fm}_{152}$. The hexacontratetrapole deformation ϵ_6 is zero for oblate shapes and is given by $\epsilon_6 = 0.2\epsilon_2$ for prolate shapes.

Fig. 91 Calculated neutron single-particle level diagram for nuclei in the vicinity of $^{252}_{100}\mathrm{Fm}_{152}$. The hexacontratetrapole deformation ϵ_6 is zero for oblate shapes and is given by $\epsilon_6 = 0.2\epsilon_2$ for prolate shapes.

Fig. 92 Calculated proton single-particle level diagram for nuclei in the vicinity of $^{262}_{100}\mathrm{Fm}_{162}$.

Fig. 93 Calculated neutron single-particle level diagram for nuclei in the vicinity of $^{262}_{100}\mathrm{Fm}_{162}$.

Fig. 94 Calculated proton single-particle level diagram for superheavy nuclei in the vicinity of $^{272}110_{162}$, which is calculated to be deformed in its ground state.

Fig. 95 Calculated neutron single-particle level diagram for superheavy nuclei in the vicinity of $^{272}110_{162}$, which is calculated to be deformed in its ground state.

Fig. 96 Calculated proton single-particle level diagram for superheavy nuclei in the vicinity of $^{298}114_{184}$, which is calculated to be spherical in its ground state.

Fig. 97 Calculated neutron single-particle level diagram for superheavy nuclei in the vicinity of $^{298}114_{184}$, which is calculated to be spherical in its ground state.

Fig. 98 Calculated proton single-particle level diagram for superheavy nuclei in the vicinity of $^{308}124_{184}$, which is calculated to be spherical in its ground state.

Fig. 99 Calculated neutron single-particle level diagram for superheavy nuclei in the vicinity of $^{308}124_{184}$, which is calculated to be spherical in its ground state.

EXPLANATION OF TABLE

Table. Calculated Nuclear Ground-State Properties

$\boldsymbol{Z}$	Proton number. The Table is ordered by increasing proton number. The corresponding chemical symbol of each named element is given in parentheses. For consistency we use the same naming scheme as in our earlier publication,[1]) although the names of some of the heavier elements may be officially changed in the future.
N	Neutron number.
A	Mass number.
$\Omega_{\rm p}^{\pi}$	Projection of the odd-proton angular momentum along the symmetry axis and parity of the wave function.
$\Omega_{\rm n}^{\pi}$	Projection of the odd-neutron angular momentum along the symmetry axis and parity of the wave function.
$\Delta_{\rm LN_p}$	Pairing gap for protons in the Lipkin-Nogami model, given by $\Delta_{\rm p} + \lambda_{\rm 2p}$.
$\Delta_{\rm LN_n}$	Pairing gap for neutrons in the Lipkin-Nogami model, given by $\Delta_{\rm n} + \lambda_{\rm 2n}$.
$E_{\rm bind}$	Total binding energy.
$S_{\rm 1n}$	One-neutron separation energy.
$S_{\rm 2n}$	Two-neutron separation energy.
P_A	Probability for producing a final nucleus with mass number A following β decay and delayed neutron emission.
P_{A-1}	Probability for producing a final nucleus with mass number $A-1$ following β decay and delayed neutron emission.
P_{A-2}	Probability for producing a final nucleus with mass number $A-2$ following β decay and delayed neutron emission.
Q_β	Energy released in β decay.
T_β	Half-life with respect to Gamow-Teller β decay.
$S_{\rm 1p}$	One-proton separation energy.
$S_{\rm 2p}$	Two-proton separation energy.
Q_α	Energy released in α decay.
T_α	Half-life with respect to α decay.

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